

INTERNATIONAL TABLES
FOR
X-RAY CRYSTALLOGRAPHY

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VOL. II. MATHEMATICAL TABLES

VOL. III. PHYSICAL AND CHEMICAL TABLES

VOL. IV. REVISED AND SUPPLEMENTARY TABLES

THE INTERNATIONAL UNION OF PURE AND APPLIED PHYSICS

IN COOPERATION WITH THE INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY

AND THE INTERNATIONAL UNION OF PURE AND APPLIED PHYSICS

AND THE INTERNATIONAL UNION OF PURE AND APPLIED PHYSICS

1962

SCI REF
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1985
Vol. 2

INTERNATIONAL TABLES FOR X-RAY CRYSTALLOGRAPHY

VOL. I. SYMMETRY GROUPS
VOL. II. MATHEMATICAL TABLES
VOL. III. PHYSICAL AND CHEMICAL TABLES
VOL. IV. REVISED AND SUPPLEMENTARY TABLES

Published for
THE INTERNATIONAL UNION OF CRYSTALLOGRAPHY
by

D. REIDEL PUBLISHING COMPANY

A MEMBER OF THE KLUWER



ACADEMIC PUBLISHERS GROUP

DORDRECHT / BOSTON / LANCASTER

1985

ISBN 90-277-1956-X

Printed in The Netherlands by
D. REIDEL PUBLISHING COMPANY
Dordrecht, Holland

<i>1st edition</i>	<i>1959</i>
<i>2nd edition, reprinted with corrections</i>	<i>1967</i>
<i>3rd edition, reprinted with corrections</i>	<i>1972</i>
<i>3rd edition, reprinted</i>	<i>1985</i>

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Volume II
MATHEMATICAL TABLES

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CONTENTS

	PAGE
1. INTRODUCTION (John Kasper)	1
1.1. Purpose and Scope of the Tables	1
1.2. Arrangement of Tables	1
1.3. Acknowledgments, etc.	1
2. FUNDAMENTAL MATHEMATICS (A. L. Patterson)	3
2.0. Introduction	5
2.1. Algebra	6
2.1.1. Complex Numbers	6
Definitions, Algebra, Applications, Examples	6
2.1.2. Series	6
2.1.2.1. Binomial Theorem	6
2.1.2.2. Multinomial Theorem	6
2.1.2.3. Progressions	7
2.1.2.4. Miscellaneous Power Series	7
2.1.3. Mathematical Constants	7
2.1.4. Linear and Rational Independence. Definitions	7
2.1.5. Modular Algebra (Algebra of Congruences)	7
2.1.6. Simple Continued Fractions	8
Table 2.1.6A. Computation Scheme for Expansion of a_1/a_2 as a Simple Continued Fraction	8
Table 2.1.6B. Expansions in Simple Continued Fractions. Examples	9
Properties of the Convergents. Examples	9
Table 2.1.6C. Table of Penultimate and Intermediate Convergents for the Ratios a_1/a_2 ($0 < a_1 < a_2 < 20$)	10
2.1.7. Determinants	11
2.1.8. Matrices	11
2.1.8.1. Definitions	11
2.1.8.2. Basic Operations	11
2.1.8.3. Determinants and Rank	12
2.1.8.4. Reciprocal Matrices	12
2.1.8.5. Characteristic Values. Example	12
2.1.8.6. Diagonalization of a Quadratic Form. Example	13
2.1.8.7. Transformation of Matrices: Elementary Operations. Equivalent Matrices and Canonical Forms	14
2.1.8.8. Differentiation of Matrices	15
2.1.8.9. Functions of a Matrix	15
2.1.8.10. Numerical Calculations with Matrices: Reduction of a Matrix	15
Table 2.1.8.10A. Reduction of a Non-singular Matrix	16
Table 2.1.8.10B. Reduction of a Singular Matrix	16
2.1.9. Linear Equations	16
2.1.9.1. Non-homogeneous Systems	16
2.1.9.2. Homogeneous Systems	17
2.1.9.3. Numerical Solution of a System of Linear Equations	17
Table 2.1.9.3A. Solution of Linear Simultaneous Equations (Five equations and four unknowns: Solution unique non-zero)	18
Table 2.1.9.3B. Solution of Linear Simultaneous Equations (Variables under-determined)	18
Table 2.1.9.3C. Solution of Linear Simultaneous Equations (Equations incompatible)	19
2.1.9.4. Solutions of Homogeneous Systems valid in a Lattice	19
Table 2.1.9.4A. System of Equations valid in a Lattice	20
Table 2.1.9.4B. Ditto. Second Example	21
Table 2.1.9.4C. Ditto. Third Example	21
2.1.10. Transcendental Equations	22
2.1.10.1. Single Variable	22

CONTENTS

2.1. Algebra (continued)	PAGE
Table 2.1.10.1A. Example of the Newton-Raphson Method	23
Table 2.1.10.1B. Example of the Rule of False Position	23
Table 2.1.10.1C. Examples of the Method of Iteration	24
2.1.10.2. Simultaneous Equations in Several Variables	24
Table 2.1.10.2. Solution of Simultaneous Transcendental Equations	24
2.1.11. Polynomial Equations	26
2.1.11.1. General Results	26
2.1.11.2. Location of Roots	26
2.1.11.3. Special Equations	26
Table 2.1.11.3. Solution of the Cubic $y^3+3Hy+G=0$	27
2.1.11.4. Horner's Reduction for a Polynomial Equation	28
Table 2.1.11.4A. Horner's Reduction	28
Table 2.1.11.4B. Use of Horner's Method in the Solution of a Polynomial Equation	28
2.1.11.5. Graeffe's Root-squaring Method	29
2.1.12. Groups	29
2.1.12.1. Group Postulates	29
2.1.12.2. Definitions	29
2.1.12.3. Results and Examples of Group Theory	30
Table 2.1.12.3. Construction of Group Multiplication Table for the Point Group 23. Notation	32
2.1.12.4. Space Groups	33
Table 2.1.12.4. Analysis of General Positions for Space Groups Isomorphous with the Point Group 222	33
2.1.12.5. Group Considerations and the Derivation of Vector Distance Sets	34
Table 2.1.12.5. Analysis of Co-ordinates and Vector Distances for the Space Group $P2_13$	35
 2.2. Trigonometry and Geometry	 36
2.2.1. Properties of Trigonometric and Hyperbolic Functions	36
2.2.1.1. Definitions	36
2.2.1.2. Functions of Multiple Angles	37
2.2.1.3. Addition Formulae and Product Formulae	37
2.2.1.4. Sums of Trigonometric Functions	37
2.2.1.5. Miscellaneous Formulae	37
2.2.1.6. Approximations for Trigonometric Functions	38
2.2.1.6.1. Least Squares Approximations	38
Table 2.2.1.6A. Ranges of Approximations for Trigonometric Functions	38
Table 2.2.1.6B. Series for Linear Interpolation for Cosine	39
2.2.1.6.2. Approximations for Sketching	39
2.2.2. Plane Trigonometry	39
2.2.2.1. Notation	39
2.2.2.2. Basic Formulae and Properties	39
2.2.2.3. Special Properties of the Plane Triangle	40
2.2.2.4. Regular Convex Polygons, n Sides	40
2.2.3. Spherical Trigonometry	40
2.2.3.1. Notation	40
2.2.3.2. Basic Formulae	40
2.2.3.3. Polar Triangles	40
2.2.3.4. Right-angled Spherical Triangles	40
2.2.3.5. Solid Angle	41
2.2.4. Plane Analytic Geometry	41
2.2.4.1. Straight Line (Intercept Equation, Slope and Intercept Equation, Perpendicular Equation, Line through Two Points, General Equation, Perpendicular Distance from a Point on to a Line, Intersection of Two Lines, Area of a Triangle of Given Vertices)	41
2.2.4.2. Curves of the Second Degree	42
Table 2.2.4.2. Reduction of General Quadratic	42
2.2.4.3. General Properties of Plane Curves	43
2.2.5. Solid Analytic Geometry	43

2.2. Trigonometry and Geometry (<i>continued</i>)	PAGE
2.2.5.1. The Plane (Intercept Equation, Perpendicular Equation, Plane through Three Points, the General Equation, Perpendicular Distance from a Point on to a Plane, Angle between Two Planes)	43
2.2.5.2. The Line (Line through Two Points, Line through One Point in a Given Direction, the General Equation of a Line, Properties of Two Lines, Volume of a Tetrahedron)	44
2.2.5.3. Surfaces of the Second Degree	44
Table 2.2.5.3. Reduction of General Conicoid	44
2.2.5.4. General Properties of Surfaces	46
2.2.5.5. Properties of Regular Solids (in collaboration with P. J. Brown and H. D. Megaw)	46
Table 2.2.5.5. Dimensions of Regular Solids: (a) Cube, (b) Tetrahedron, (c) Octahedron, (d) Rhombic Dodecahedron, (e) Regular (pentagonal) Dodecahedron, (f) Isosahedron, (g) Cuboctahedron	46
2.3. Differential and Integral Calculus	50
2.3.1. Differential Calculus. Definitions and Notations, Basic Forms, Derivatives of Simple Functions, Taylor's Series, Differentiation of an Integral	50
2.3.2. Integral Calculus	51
2.3.2.1. Indefinite Integrals	51
2.3.2.2. Definite Integrals	51
2.4. Vector and Tensor Analysis	52
2.4.1. Definitions	52
2.4.2. Absolute Vector Analysis	52
2.4.3. Base Systems and their Reciprocal Systems	53
2.4.3.1. Summation Convention	53
2.4.3.2. General Base Systems	53
2.4.3.3. Cartesian Base Systems	53
2.4.3.4. Cylindrical and Polar Co-ordinates	53
2.4.3.5. The Physical Dimensions associated with Base Systems	54
2.4.4. Tensor Analysis	54
Table 2.4.4. Properties of Base and Reciprocal Systems	57
2.4.5. Dyadics	57
Table 2.4.5. Dyadics for the Crystallographic Proper Rotations	58
2.4.6. Parallelism between Matrix, Tensor and Dyadic Notations for a Second Order Tensor ..	59
Table 2.4.6A. Comparison between Tensor, Dyadic and Matrix Notations	59
Table 2.4.6B. Matrix Transformations for Second Order Tensor	59
2.4.7. Vector and Tensor Problems in Crystal Analysis	60
2.4.7.1. Calculations of Bond Lengths and Bond Angles	60
Table 2.4.7A. Metric Tensors for Crystal Lattices	60
2.4.7.2. Numerical Example of the Calculation of Bond Lengths and Bond Angles	61
2.4.7.3. Rotations	62
Table 2.4.7B. Cartesian Rotation Matrices for the Crystallographic Axes	63
2.5. Fourier Theory	65
2.5.1. Orthogonal Functions	65
2.5.2. The Delta Function	66
2.5.3. Fourier Transforms	66
2.5.3.1. Basic Mathematics	66
2.5.3.2. Evaluation of Fourier Transforms	67
Table 2.5.3A. Properties of Fourier Transforms	68
Table 2.5.3B. Some Fourier Transforms	69
2.5.3.3. Fourier Transforms in Two and Three Dimensions	71
Table 2.5.3C. Properties of Three-dimensional Transforms	71
Table 2.5.3D. Some Three-dimensional Fourier Transforms	72
2.5.3.4. Evaluation of Three-dimensional Fourier Transforms	73
2.5.4. Fourier Series	73
2.5.4.1. Basic Theory	73
2.5.4.2. Fourier Transform of a Periodic Function	73

	PAGE
2.5. Fourier Theory (continued)	
Table 2.5.4A. <i>Properties of Fourier Series</i>	74
2.5.4.3. Fourier Series for an Arbitrary Period	74
2.5.4.4. Calculation of Fourier Coefficients	75
2.5.4.5. Numerical Calculations for Fourier Series	75
Table 2.5.4B. <i>Some Fourier Series</i>	76
2.5.4.6. Fourier Series in Two Dimensions	78
2.5.4.7. Expansion of Two-dimensional Series in Terms of One-dimensional Series	78
2.5.4.8. Symmetry of the Beevers-Lipson Expansion, with Three Examples	79
Table 2.5.4C. <i>Symmetry and Antisymmetry Properties of Beevers-Lipson Summation</i>	80
2.5.4.9. Fourier Series in Three Dimensions	80
2.5.4.10. Properties of Convolutions	81
Table 2.5.4D. <i>Forms for the Convolution Formulae</i>	82
Table 2.5.4E. <i>Forms for Auto-convolutions</i>	82
Table 2.5.4F. <i>Convolutions of "Atomic Functions"</i>	83
2.6. Statistics (D. W. J. Cruickshank)	84
2.6.1. Introduction	84
2.6.1.1. General Introduction	84
2.6.1.2. Fundamental Rules for Combining Probabilities	84
2.6.2. One-dimensional Probability Distributions	84
2.6.2.1. Discrete and Continuous Distributions	84
2.6.2.2. Moments	85
2.6.2.3. Measures of Location	85
2.6.2.4. Measures of Dispersion	85
2.6.2.5. Measures of Skewness	85
2.6.2.6. Characteristic Functions	86
2.6.3. Particular One-dimensional Distributions	86
2.6.3.1. The Binomial Distribution	86
2.6.3.2. Poisson's Distribution	87
2.6.3.3(a). The Normal Distribution	87
2.6.3.3(b). The Central Limit Theorem	87
2.6.3.4. The χ^2 Distribution	87
2.6.3.5. The t Distribution, or Student's Distribution	87
2.6.3.6. The F and z Distributions	88
2.6.4. Multi-dimensional Distributions	88
2.6.4.1(a). Two-dimensional Probability Distributions	88
2.6.4.1(b). Regression Curves	88
2.6.4.2. Multi-dimensional Probability Distributions	88
2.6.5. Sampling Distributions	89
2.6.5.1. Large Samples	89
2.6.5.2. Sheppard's Corrections	89
2.6.5.3. Small Samples	90
2.6.6. Statistical Inference	90
2.6.6.1. One-dimensional Confidence Intervals	90
2.6.6.2. One-parameter Significance Tests	90
2.6.6.3. Weighted Mean Values and the Detection of Systematic Errors	91
2.6.6.4. The Method of Least Squares	92
2.6.6.5. Multi-parameter Confidence Regions and Significance Tests	94
2.6.6.6. χ^2 as a Test of Goodness of Fit	94
Table 2.6.6A. <i>The Significance Points t_p of the t Distribution</i>	94
Table 2.6.6B. <i>The Significance Points χ_p^2 of the χ^2 Distribution</i>	95
General References	96
Special References	97
3. CRYSTAL GEOMETRY (J. D. H. Donnay and Gabrielle Donnay)	99
3.1. General Relations, valid for all Crystal Systems	101
3.1.1. Definition of Terms	101

3.1. General Relations, valid for all Crystal Systems (<i>continued</i>)	PAGE
3.1.2. Direct and Reciprocal Lattices	101
3.1.3. The Row Line	101
3.1.4. The Net Plane	102
3.1.5. Fundamental Formula	102
3.1.6. Relations between Nets and Rows in One and the Same Space	102
3.1.7. Relations between Planes in Direct Space and Rows in Reciprocal Space, and vice versa	103
3.1.8. Formulae of Miller	103
3.1.8.1. Direct Sine Formula	103
3.1.8.2. Converse Cotangent Formula	103
3.1.8.3. Harmonic Case	103
3.1.9. Twinning	104
3.1.9.1. Introduction	104
3.1.9.2. Graphical Determination of the Rotations	104
3.1.9.3. Analytical Determination of the Rotations	104
3.1.9.4. Choice of Twin Law	104
3.1.9.5. Twin Obliquity	104
3.1.9.6. Twin Index	105
<i>Table 3.1.9. Twin Index in Terms of $S= hu+kv+lw$</i>	105
3.2. Triclinic System	106
3.2.1. Cell	106
3.2.2. Direct Lattice	106
3.2.3. Reciprocal Lattice	106
3.2.4. Choice of Direct Cell	106
3.2.5. Interplanar Angle	106
3.2.6. Quadratic Form Q and Interplanar Distance d	106
3.2.7. Twinning	106
3.2.7.1. Only One Possible Rotation	106
3.2.7.2. Perpendicularity Condition	106
3.2.7.3. Twinning Condition	106
3.3. Monoclinic System	107
3.3.1–3.3.7. As before.	
3.3.7.1. Two Possible Rotations	107
3.3.7.2. Perpendicularity Condition	107
3.3.7.3. Twinning Condition	107
3.4. Orthorhombic System	108
3.4.1–3.4.7. As before.	
3.4.7.1. Four Possible Rotations	108
3.4.7.2. Perpendicularity Condition	108
3.4.7.3. Twinning Condition	108
3.5. Tetragonal System	109
3.5.1–3.5.7. As before.	
3.5.7.1. Eight Possible Rotations	109
3.5.7.2. Perpendicularity Condition	109
3.5.7.3. Twinning Condition	109
<i>Table 3.5.5. Interplanar Angles in the Tetragonal Zone. $\phi=(010):(hk0)$, $h < k$</i>	109
<i>Table 3.5.6. Tetragonal Quadratic Forms. Given h^2+k^2, to find h and k</i>	110
3.6. Hexagonal System (<i>Sensu lato</i>, including trigonal). Hexagonal Axes $xyuz$ and Bravais-Miller 4-index Symbols $hkil$, with $i=-(h+k)$	112
3.6.1–3.6.5. As before.	
<i>Table 3.6.5. Interplanar Angles in the Hexagonal Zone. $\phi=(11.0):(hk.0)$, $h > k$</i>	112
<i>Table 3.6.6. Hexagonal Quadratic Forms. Given h^2+k^2+hk, to find h and k</i>	113
3.6.6. Quadratic Form Q and Interplanar Distance d	115
3.6.7. Twinning	115
3.6.7.1. Twelve Possible Rotations	115
3.6.7.2. Perpendicularity Condition, with note about Weber 4-index symbol	115
3.6.7.3. Twinning Condition	115

CONTENTS

	PAGE
3.7. Rhombohedral System (<i>Sensu stricto</i> , trigonal crystals with rhombohedral lattice). Rhombohedral	116
Axes and Miller 3-index Symbols	116
3.7.1–3.7.7. As before.	
3.7.7.1. Six Possible Rotations	116
3.7.7.2. Perpendicularity Condition	116
3.7.7.3. Twinning Condition	116
Table 3.7.6. <i>Rhombohedral Quadratic Forms. Given $h^2+k^2+l^2$, to find hkl and $kl+lh+hk$</i>	117
3.8. Cubic System	119
3.8.1–3.8.5. As before.	
Table 3.8.5A. <i>Number of Distinct Interplanar Angles between any Given Plane and all the Faces of a Given Form</i>	119
Table 3.8.5B. <i>Cubic Interplanar Angles</i>	120
3.8.6. Quadratic Form Q and Interplanar Distance d	123
3.8.7. Twinning	123
3.8.7.1. Twenty-four Possible Rotations	123
3.8.7.2. Perpendicularity Condition	123
3.8.7.3. Twinning Condition	123
Table 3.8.6A. <i>Cubic Quadratic Forms. $s=h^2+k^2+l^2$, \sqrt{s} and mantissa of $\log s$; hkl</i>	124
Table 3.8.6B. <i>Space Groups in Each of the 17 Cubic Aspects</i>	147
Table 3.8.6C. <i>Reflections permitted by Each of the 17 Cubic Aspects</i>	147
3.9. Hexagonal-rhombohedral Transformations (A. Pabst)	150
3.9.1. Transformation of Cell Constants	150
3.9.2. Transformation of Indices. Example	150
Table 3.9.1. <i>Hexagonal and Rhombohedral Constants</i>	152
Table 3.9.2. <i>Hexagonal-to-Rhombohedral Transformation of Indices</i>	156
General and Special References	158
 4. DIFFRACTION GEOMETRY (H. T. Evans, Jr., and K. Lonsdale)	 159
4.1. Classification of Diffraction Methods	161
Table 4.1.1. <i>Classification of the Main X-ray Diffraction Techniques</i>	161
4.2. Fixed-crystal Methods	164
4.2.1. Laue Method	164
4.2.1.1. Plane Film: polar stereographic net, Wulff net, gnomonic net, Greninger chart	164
Table 4.2.1.1A. <i>Table for Conversion of Front-reflection Laue Patterns to Stereographic or Gnomonic Projections</i>	165
Table 4.2.1.1B. <i>Table for Conversion of Back-reflection Laue Patterns to Stereographic or Gnomonic Projections</i>	166
4.2.1.2. Cylindrical Film	167
Table 4.2.1.2. <i>Tables for Conversion of Cylindrical Laue Patterns to Stereographic Projections</i>	168
4.2.2. Divergent-beam Method	174
4.3. Moving Single-crystal Methods	175
4.3.1. Symbols in Use	175
Table 4.3.1. <i>Symbols used to specify Quantities on Diffraction Patterns and in Reciprocal Space</i>	175
4.3.2. Relationships between Cylindrical Co-ordinates ϕ , ξ , ζ of Reciprocal-lattice Point P and the Position of the Corresponding Diffraction Spot	175
4.3.2.1. General Case	175
4.3.2.2. Diffraction observed on Sphere	176
4.3.2.3. Diffraction observed on Plane Film	177
4.3.2.4. Cylindrical Stationary Film; Crystal on Axis; Crystal on Circumference	177
4.3.2.5. Alternative Expressions for ζ and ξ	178
Table 4.3.2. <i>Co-ordinates for Construction of Bernal Chart</i>	180
4.3.3. Identity Distances on Stationary Films	179
4.3.4. Indexing of Zero-layer Line	184
Table 4.3.4. <i>Data for Bunn Chart for Indexing of Rotation Zero Line</i>	182

	PAGE
4.4. Weissenberg Method	185
4.4.1. Experimental Details	185
4.4.2. Interpretation of Weissenberg Patterns	185
Table 4.4.1A. <i>Equi-inclination Weissenberg Method Setting Constants</i>	187
Table 4.4.1B. <i>Normal-beam and Flat-cone Weissenberg Methods Setting Constants</i>	189
Table 4.4.2A. <i>Data for Nomogram for Conversion of Equi-inclination Weissenberg Film Co-ordinates to Reciprocal-lattice Cylindrical Co-ordinates</i>	190
Table 4.4.2B. <i>Data for Row-line Indexing Chart for Weissenberg Equi-inclination Photographs</i>	192
4.5. Buerger Precession Method	194
Table 4.5.1. <i>Layer-screen Settings for Zero-level Photographs with the Buerger Precession Camera</i>	194
Table 4.5.2. <i>Data for setting the Buerger Precession Camera for Upper Levels</i>	195
Table 4.5.3. <i>Reciprocal-lattice Layer Heights from Cone-axis Photographs with the Buerger Precession Camera</i>	197
Table 4.5.4. <i>Data for Construction of Buerger Precession Setting Nomogram</i>	198
Table 4.5.5. <i>Angular Setting Error in Terms of Displacement of Zero-level Lattice Plane on the Buerger Precession Photograph</i>	200
Table 4.5.6. <i>De Jong and Bouman Method Setting Constants</i>	201
4.6. Random-orientation Methods	202
4.6.1. Indexing Powder Patterns, given Lattice Constants	202
4.6.2. Determining Unknown Lattice Constants	203
Table 4.6. <i>Quick-reference Table of d (Spacings) vs. Bragg Angle for Various Mean Wavelengths</i>	204
Table 4.6.2A. <i>Data for Construction of Bunn Chart for indexing Tetragonal Powder Patterns</i>	207
Table 4.6.2B. <i>Similar Data for Hexagonal Powder Patterns</i>	212
4.7. Precision Measurement of Lattice Parameters of Polycrystalline Specimens (W. Parrish and A. J. C. Wilson)	216
4.7.1. Introduction	216
4.7.2. Photographic Methods	216
4.7.2.1. <i>Debye-Scherrer Method</i>	217
Table 4.7.2.1. <i>Systematic Errors in the Debye-Scherrer Method</i>	218
4.7.2.2. <i>Symmetrical Back-reflection Focusing Method</i>	218
Table 4.7.2.2. <i>Systematic Errors in the Symmetrical Back-reflection Focusing Method</i>	219
Table 4.7.2.3. <i>Corrections to Measurements with Flat-plate Back-reflection Camera</i>	219
4.7.2.3. <i>Flat-plate Back-reflection Method</i>	220
4.7.3. Counter-diffractometer Method	220
Table 4.7.3. <i>Sources of Major Errors in Counter Diffractometry</i>	221
4.7.4. General Problems: extrapolation; thermal expansion; refraction; X-ray wavelengths	225
Table 4.7.4A. $\frac{1}{2} \left(\frac{\cos^2 \theta}{\sin \theta} + \frac{\cos^2 \theta}{\theta} \right)$ vs. θ° (10 to 89 by 0.1)	228
Table 4.7.4B. $\sin^2 \theta$ and $\cos^2 \theta$ vs. θ° (0 to 90 by 0.01)	230
Table 4.7.4C. $\phi \tan \phi$ vs. ϕ° (0 to 45 by 0.1)	232
General and Special References	233
5. PHYSICS OF DIFFRACTION METHODS (H. Lipson)	235
5.1. Basic Definitions and Formulae	237
5.1.1. <i>Definitions of Symbols</i>	237
5.1.2. <i>Formulae for Scattering by an Electron</i>	237
5.1.3. <i>Formula for the Atomic Scattering Factor f_0</i>	237
Table 5.1.2. <i>Polarization Factor, $p = \frac{1 + \cos^2 2\theta}{2}$, as a Function of $\sin \theta$</i>	238
5.2. Intensity of Radiation Diffracted by a Crystal	241
5.2.1. <i>Structure Factor</i>	241
5.2.2. <i>Temperature Factor</i>	241
Table 5.2.2A. $\exp(-B \sin^2 \theta / \lambda^2)$: $(\sin \theta) / \lambda$ 0.01 to 1.50 by 0.01, B 0.1 to 10.0 by 0.1	242

5.2. Intensity of Radiation Diffracted by a Crystal (*continued*)

PAGE

Table 5.2.2B. Values of $\phi(x) = \frac{1}{x} \int_0^x \frac{\xi}{e^\xi - 1} d\xi$ as a Function of x	264
5.2.3. Integrated Reflection (a) from a crystal element, (b) from an extended crystal face ..	265
5.2.4. Correction of Intensities for Angle Factors	265
5.2.4.1. Single Crystal: Beam Normal to Rotation Axis	265
5.2.4.2. Single Crystal: Equi-inclination Weissenberg Photograph	266
5.2.4.3. Debye-Scherrer Lines on Cylindrical Film	266
5.2.5. Lorentz-polarization Factors	266
5.2.5.1. Normal-beam Method, $\mu=0$	266
5.2.5.2. Equi-inclination Method, $\mu=-\nu$	266
5.2.5.3. The Precession Method (C. E. Nordman)	267
5.2.5.4. Other Methods of Recording	267
5.2.5.5. General Remarks on the Use of Charts and Tables	267
Table 5.2.5A. Lorentz-polarization Factor, $2Lp = \frac{1 + \cos^2 2\theta}{\sin 2\theta}$ as a Function of $\sin \theta$	268
Table 5.2.5B. Correcting Factor $\frac{4Lp}{\sin \theta} = \frac{1 + \cos^2 2\theta}{\sin^2 \theta \cos \theta}$ as a Function of $\sin \theta$	270
Table 5.2.5C. Correcting Factor $\frac{4Lp}{\cos \theta} = \frac{1 + \cos^2 2\theta}{\sin \theta \cos^2 \theta}$ as a Function of $\sin \theta$	272
Table 5.2.5D. Data for the Construction of Constant $(Lp)^{-1}$ Curves for Rotation and Oscillation Photographs	274
Table 5.2.5E. Values of ξ , for a Range of Values of ζ , at which $(Lp)^{-1}$ assumes the Values 0, 0.1, 0.2, . . . , 2.0	275
Table 5.2.5F. Data for the Construction of Constant $(Lp)^{-1}$ Curves for Equi-inclination Weissenberg Photographs	276
Table 5.2.5G. Values of ξ , for a Range of Values of ζ , at which $(Lp)^{-1}$ assumes the Values 0, 0.1, 0.2, . . . , 2.0	277
Table 5.2.5H. Lorentz-polarization Corrections for the Precession Method, $\bar{\mu}=30^\circ$ (C. E. Nordman) ..	278
Table 5.2.5I. $(Lp)^{-1}$ for Zero-level Precession Photographs, for Odd Values of $\bar{\mu}$ 11° to 29° (J. Kraut) ..	286
5.3. Absorption Corrections. (a) Small Crystal bathed in Narrow Beam. (b) Large Crystal or Crystal-line Powder Block intercepting the Entire Narrow Beam	291
5.3.1. Reflection of Narrow Beam from Planes Parallel to Extended Face of Crystal: (a) Crystal of Sufficient Thickness to give Negligible Transmission. (b) Transmission not Negligible, Crystal Thickness t	291
5.3.2. Reflection from Crystal Planes inclined at Angle ϕ to Extended Face of Crystal Block of Negligible Transmission	291
5.3.3. Transmission when the Reflecting Planes are Perpendicular to the Surfaces of the Block, of Thickness t	291
5.3.4. Transmission when the Reflecting Planes are inclined at an Angle $(\pi/2) - \phi$ to the Surfaces of the Block of Thickness t	291
5.3.5. Cylindrical Crystal of Radius R , bathed in a Uniform Beam of X-rays Normal to its Axis (W. L. Bond)	291
5.3.5.1. Method based on Automatic Computation	291
5.3.5.2. Modification for Large Values of μR (>8)	292
Table 5.3.5A. Calculation of Transmission Factor A for Cylinder, Radius R (W. L. Bond)	292
Table 5.3.5B. Absorption Correction Factors A^* for Successive Values of θ (W. L. Bond)	295
Table 5.3.5C. Alternative Method of Calculating Transmission Factor A (W. L. Bond)	299
5.3.5.3. Upper Levels of Equi-inclination Weissenberg Photographs	299
5.3.5.4. Optimum Size of a Cylinder	299
5.3.6. Sphere of Radius R , bathed in a Uniform Incident X-ray Beam (W. L. Bond)	299
Table 5.3.6A. Transmission Factor A for Sphere, Radius R (W. L. Bond)	300
5.3.6.1. Optimum Size of Spheres	300
5.3.7. Crystal of any Shape, bathed in Uniform Beam of X-rays (A. Hargreaves)	300
5.3.8. Absorption Corrections in X-ray Examinations of Preferred Orientation in Flat Sheet Specimens (B. F. Decker)	301
Table 5.3.6B. Absorption Correction Factors A^* for Successive Values of θ . Sphere of Radius R (W. L. Bond)	302

5.3. Absorption Corrections (<i>continued</i>)	PAGE
5.3.8.1. Transmission Case: Flat Sheet Specimen	306
5.3.8.2. Reflection Case: Flat Sheet Specimen	306
Table 5.3.8. Intensity Correction Factors for X-ray Spectrometer	307
5.4. Mosaic Theory	313
5.4.1. Distinction between Perfect and Ideally Imperfect Crystals	313
5.4.2. Primary Extinction	313
Table 5.4.2. Primary Extinction Correction Factor	313
5.4.3. Secondary Extinction	313
5.5. Summary of Formulae for Integrated Intensities:	
(a) Crystal Element. (b) Crystal Face. (c) Crystal Section of Thickness t . (d) Powder Halo. (e) Debye-Scherrer Lines on Cylindrical Film. (f) Reflection from a Thick Block of Powdered Crystal of Negligible Transmission. (g) Transmission through Block of Powdered Crystal of Thickness t . (h) Rotation Photograph of Small Crystal, Volume V	314
References	315
6. FOURIER SYNTHESIS AND STRUCTURE FACTORS (D. W. J. Cruickshank)	317
6.1. Formulae for Three-dimensional Electron Density and Patterson Functions (in collaboration with G. S. Parry)	318
6.1.1. Electron Density	318
6.1.2. The Patterson Function	318
6.2. Formulae for Fourier Series, Sections, Lines, Projections and Derivatives (in collaboration with G. S. Parry)	319
6.2.1. Electron Density Sections	319
6.2.1.1. For a Plane parallel to (001)	319
6.2.1.2. For a Plane parallel to $(h_1k_1l_1)$	319
6.2.2. Electron Density Lines	319
6.2.2.1. Line parallel to [001]	319
6.2.2.2. Line parallel to $[uvw]$	319
6.2.3. Electron Density Projections	319
6.2.3.1. Whole Unit Cell projected along [001] on to any Plane not containing [001]	319
6.2.3.2. Projection along $[uvw]$ of Whole Unit Cell having $[uvw]$ as One Axis	319
6.2.3.3. Bounded Projection along [001]	320
6.2.3.4. Projection of a Number of Parallel Sections	320
6.2.3.5. Projection of Unit Cell in Planes on to a Line not parallel to the Planes	320
6.2.4. Differential Syntheses	320
6.3. Fourier Transforms	322
6.3.1. Radial Electron Densities	322
6.3.2. Diffraction Effects	322
Table 6.3.2. Values of $2r(\sin \theta_{\max})/\lambda$ for the First Four Zeros of the Diffraction Density Functions in 3, 2 and 1 Dimensions corresponding to an Atom having Unit Scattering Factor	322
6.3.3. Various Space Transforms	323
6.3.3.1. Scattering Factor for a Distribution with Spherical Symmetry	323
6.3.3.2. Scattering Factor for a Plane Distribution of Circular Symmetry	323
6.3.3.3. Scattering Factor for a Line Distribution	323
6.3.3.4. Scattering Function for a Distribution of Cylindrical Symmetry	323
6.3.3.5. Scattering Function for a Spherical Atom freely rotating Spherically	323
6.3.3.6. Scattering Function for a Spherical Atom rotating about an Axis	324
6.3.3.7. Scattering from a Hindered Rotator	324
6.3.3.8. Scattering Function for an Exponentially Decreasing Density Distribution	324
6.3.3.9. Scattering Function for a Gaussian Density Distribution	324
6.3.3.10. Transform of an Infinite Helix	324
6.3.4. Molecular Transforms	324
6.3.5. Transforms of Crystal Shapes	325
Table 6.3.5. Shape Transforms	325

	PAGE
6.4. Refinement of Structure Parameters	326
6.4.1. Application of the Method of Least Squares	326
6.4.1.1. Normal Equations	326
6.4.1.2. Values of $\partial F_c(hkl) /\partial u_j$: Atomic Co-ordinates, Isotropic Thermal Parameters, Anisotropic Thermal Parameters, Scale Factor	326
6.4.1.3. Choice of Weights	328
6.4.1.4. Approximate Equations	328
6.4.2. Refinement using Observed and Calculated Fourier Syntheses in Conjunction, or by Difference Syntheses	328
6.4.2.1. Introduction	328
6.4.2.2. General Co-ordinate Refinement Equations	329
6.4.2.3. Approximate Co-ordinate Refinement Equations, Centrosymmetric Space Groups	329
6.4.2.4. Booth's Back-shift Method for Finite Series Correction	330
6.4.2.5. Approximate Co-ordinate Equations and the "n-Shift Rule," Non-centrosymmetric Space Groups	330
6.4.3. Standard Deviations of Structure Parameters	330
6.4.3.1. Least Squares	330
6.4.3.2. Fourier Methods	331
6.4.3.3. Bond Length and Bond Angle Standard Deviations	331
6.4.4. The Discrepancy Index (or Residual)	332
6.5. The Practical Evaluation of Fourier Series and Structure Factors (in collaboration with G. A. Jeffrey and P. J. Wheatley)	333
6.5.1. The Fourier Strip Methods	333
6.5.1.1. The Beevers-Lipson Strip Method	334
6.5.1.2. The Patterson-Tunell Strip and Stencil Method	334
6.5.1.3. Robertson's Modified Strip and Stencil Method	335
6.5.2. The Bragg-Lipson Charts	335
6.5.3. Mechanical and Electromechanical Methods	335
6.5.3.1. Fourier Synthesizers	335
6.5.3.2. Structure Factor Calculators	335
6.5.4. Optical Methods	335
6.5.4.1. The Huggins Masks	335
6.5.4.2. The v. Eller "Photosommateur"	335
6.5.4.3. The X-ray Microscope	336
6.5.4.4. The Analogue Diffraction Spectrometer	336
6.5.5. Large-scale Computing Equipment	336
6.5.5.1. Computing Methods	336
6.5.5.2. Lists of Programs	336
6.5.5.3. Test Calculations	336
References	338
7. SPECIAL TOPICS	341
7.1. Close Packing (A. L. Patterson and J. S. Kasper)	342
7.1.1. Introduction	342
7.1.2. Close Packing in the Plane	342
Table 7.1.2. <i>Some Close-packed Plane Arrangements of Circles</i>	342
7.1.3. Close Packing in Space	342
Table 7.1.3. <i>Some Close-packed Space Arrangements of Spheres</i>	343
7.1.4. Closest Packing of Spheres	343
7.1.5. Symmetrical Closest-packed Stacking of Closest-packed Planes	343
Table 7.1.5A. <i>Interlayer Translations and Locations of Voids</i>	344
Table 7.1.5B. <i>Symmetry of Stacked Closest-packed Layers, with Examples</i>	344
7.1.6. Structures related to Closest Packing	349
7.1.7. Radial Distribution of Atoms	349

7.1. Close Packing (continued)	PAGE
Table 7.1.7A. Radial Distribution of Atoms in the Three Cubic Lattices	349
Table 7.1.7B. Simple Cubic	350
Table 7.1.7C. Body-centred Cubic	351
Table 7.1.7D. Face-centred Cubic	352
Table 7.1.7E. Hexagonal Closest Packing	353
References	354
7.2. The Use of Statistical Methods for the Detection of Symmetry Elements (V. Luzzati)	355
7.2.1. Determination of the Absolute Scale and of the Thermal Vibration Factor	355
Table 7.2.1A. Intensity-distribution Effects of Symmetry Elements not causing Systematic Absences	355
Table 7.2.1B. Intensity-distribution Effects of Symmetry Elements causing Systematic Absences	356
7.2.2. Detection of a Centre of Symmetry: Variance Test; Zero Moment Test	356
Table 7.2.2. Theoretical Values of the Function $N(z)$ for Centrosymmetric and Non-centrosymmetric Cases	357
References	357
7.3. Inequality Relations between Structure Factors (J. Bouman)	358
Table 7.3.1. Fundamental Set—Centre of Symmetry	358
Table 7.3.2. Derived Inequalities—Centre of Symmetry	358
Table 7.3.3. Non-centrosymmetric Structures: Fundamental Set and Derived Inequalities	358
Numerical and Graphical Examples	359
Table 7.3.4. Values of $S_{H+H'}$ and $S_{H-H'}$	359
References	360
8. MISCELLANEOUS EXPONENTIAL AND TRIGONOMETRIC TABLES	361
Table 8.1. The Exponential Function e^{-x}	362
8.2. A Four-place Table of $\frac{\sin x}{x}$ (J. Sherman, assisted by L. Brockway)	366
Table 8.2. A Four-place Table of $\frac{\sin x}{x}$	366
Table 8.3. A Short Table of $\sin 2\pi x$; $\cos 2\pi x$	379
Table 8.4. Table of Products $\left\{\frac{\cos}{\sin}\right\} 2\pi x \left\{\frac{\cos}{\sin}\right\} 2\pi y$	380
Table 8.5. Table of $\sin 2\pi hx$; $\cos 2\pi hx$	382
8.6. Conversion of Degrees to Radians, etc.	430
Table 8.6. Conversion of Degrees, Minutes and Seconds to Radians, and of Minutes and Seconds to Decimals of a Degree; and vice versa	430
9. DICTIONARY OF CRYSTALLOGRAPHIC TERMS FOR VOLUME II	433
9.1. Greek Alphabet	435
9.2. Russian Alphabet	435
9.3. Dictionary of Crystallographic Terms in English, French, German, Russian and Spanish	436
9.3.1. List of Terms in English which are similar (or easily recognizable) in all the Five Languages	436
9.3.2. List of Terms which are similar (or easily recognizable) in English, French, German and Spanish (English and Russian equivalents only are given)	438
9.3.3. List of other English Terms used in Volume II, with Equivalents in French, German, Russian and Spanish	439

LIST OF FIGURES

- Fig. 2.2.1.1. Right-angled triangle: notation
- Fig. 2.2.2.1. Plane triangle
- Fig. 2.2.3.4(1). Spherical triangle. C a right angle (Napier's Rules)
- Fig. 2.2.3.4(2). Spherical triangle. c a right angle (Napier's Rules)
- Fig. 2.5.4. Correlation between functions related by crystallographic symmetry operations
- Fig. 2.6.2.5. Continuous distribution exhibiting positive skewness
- Fig. 3.1.3. Row $[uvw]$ normal to reciprocal net $(uvw)^*$
- Fig. 3.1.4. Net (hkl) and reciprocal row $[hkl]^*$ normal to it
- Fig. 3.9.1. Correlation of axial elements and angles of rhombohedral and hexagonal cells
- Fig. 4.2.1.1(1). Geometrical principles of the spherical, stereographic, gnomonic and Laue projections
- Fig. 4.2.1.1(2). Greninger chart
- Fig. 4.2.1.2(1). Geometrical principles of Laue photography on to a cylindrical film with axis normal to the incident beam
- Fig. 4.2.1.2(2). Stereographic projection of reflecting planes giving Laue spot at angle θ , ϕ
- Fig. 4.2.1.2(3). Chart for Laue photograph on cylindrical film
- Fig. 4.3.2.1. Geometrical principles of reflection in the reciprocal lattice for the general case of a crystal rotating about an axis not necessarily normal to the incident beam
- Fig. 4.3.2.3(1). Geometrical principles of photography on to plane film normal to trace of incident beam on equatorial plane
- Fig. 4.3.2.3(2). Case where film makes an angle α in the equatorial plane with the trace of the incident beam
- Fig. 4.3.2.4(1). Geometrical principles of photography on to a cylindrical film
- Fig. 4.3.2.4(2). Crystal on circumference of cylinder (Seemann-Bohlin method)
- Fig. 4.3.2.4(3). Bernal chart for cylindrical camera
- Fig. 4.3.4. Bunn chart for indexing an orthogonal net from the zero row of a rotation photograph
- Fig. 4.4.2(1). Nomogram for transforming Weissenberg film co-ordinates to cylindrical reciprocal-lattice co-ordinates
- Fig. 4.4.2(2). Equi-inclination Weissenberg transform of parallel lattice rows
- Fig. 4.5.4. Nomogram for determination of setting constants of the Buerger precession camera for photographing a given lattice plane
- Fig. 4.5.5. Appearance of disoriented zero-level lattice plane on Buerger precession orientation photograph
- Fig. 4.6.2(1). Layout of Bunn chart for indexing tetragonal powder photographs
- Fig. 4.6.2(2). Layout of Bunn chart for indexing hexagonal powder photographs
- Fig. 4.7.1. Percentage precision of d as a function of reflection angles for various errors $\Delta 2\theta$
- Fig. 4.7.3(1). Flat specimen aberration shown by change of intensity distribution
- Fig. 4.7.3(2). Shift of centre of gravity due to flat-specimen aberration
- Fig. 4.7.3(3). Shift of centre of gravity due to specimen-transparency aberration
- Fig. 4.7.3(4). Change in line profile caused by increasing divergence of beam in plane of parallel slits
- Fig. 5.3.7. Absorption in crystal of any shape
- Fig. 5.3.8(1). Flat sheet specimen: transmission case
- Fig. 5.3.8(2). Special case for counter technique: transmission case
- Fig. 5.3.8(3). Special case for counter technique: reflection case
- Fig. 6.3.2. Curves of density functions
- Fig. 7.2.2. Comparison of centrosymmetric and non-centrosymmetric intensity distributions
- Fig. 7.3.1. Graph to determine signs of $U_{H+H'}$ and $U_{H-H'}$

PREFACE TO THE 1972 EDITION

In this edition the Corrigenda on pages xix and xx of the 1967 Edition have all been incorporated in the text. In addition, a few other corrections and changes have been made in the present text and some (un-numbered) new references have been added. It is intended to publish in *Acta Crystallographica* a consolidated list of all changes made in the various editions of the several volumes of the *Tables*.

Section 6.5.5 on Large-scale Computing Equipment has been entirely replaced by a summary account with new numbered references and mention has been made of the new Volume IV which contains some sections relevant to computing problems.

1. INTRODUCTION

JOHN KASPER

1.1. Purpose and Scope of the Tables

The present Volume contains information primarily of a mathematical nature and is characterized by the absence of physical data, which are compiled in Volume III. It comprises tables of functions, formulae and geometrical diagrams that for the most part are strictly mathematical, even though they may pertain to the application of a physical effect (for example, a table of $\exp[-B(\sin \theta/\lambda)^2]$ is given for applying the effect of temperature motion on diffracted intensities). There are included, as well, general relationships between physical quantities, but essentially none of the material is of a kind to require revision on the basis of improved physical measurements.

It is intended that this Volume should be useful in many stages of a crystal-structure determination: in the recording of X-ray diffraction effects; in the indexing of the recorded diffraction data; in the correction of intensities for geometrical and physical factors; in the production of vector and electron-density maps; and in the calculation of structure factors. Appropriate material is provided also for various other aspects of crystallographic research and the utilization of X-ray diffraction effects. A special feature is the inclusion of a comprehensive compilation of basic mathematics. This should serve a dual purpose: a utilitarian one is that of providing those simple items of mathematics which may occur in standard handbooks and texts but to which the crystallographer needs to make frequent reference; a second aim is to make available in a uniform treatment those mathematical topics that are basic to theoretical structure work but which occur in a scattered way, often with different notations, in a very extensive literature.

1.2. Arrangement of Tables

The decision on the division of the contents into the various sections and on the placement of the tabular material has been made on the basis of affording maximum convenience in the use of the Volume. In practice, at a given stage of a structure investigation one usually needs to consult only the material of one of the sections. The section headings themselves suggest the nature of their contents and the aspect of structure work to which they are applicable.

It seemed natural to have the basic mathematics

(Section 2) precede all other material. Crystal geometry (Section 3) contains subject matter conventionally associated with the title. It includes the quadratic forms which are required for deducing interplanar spacings and for indexing powder patterns. The section has been subdivided according to crystal system, since generally one will wish to consult it in regard to one particular crystal or substance. Sections 4 and 5 have to do with diffraction methods and effects; Section 4 is principally concerned with the recording of data; Section 5 with the various factors modifying the intensity of a diffracted beam. The special role of Fourier methods in crystal-structure problems makes desirable a separate Section 6 devoted to them. Three special topics are classified separately in Section 7. Finally, the extensiveness of the tables of $\sin 2\pi hx$ and $\cos 2\pi hx$ has made it seem worth while to include them along with other trigonometric and exponential tables separately as Section 8, in the convenient location of the final pages of the book.

The accuracy and reliability of the various tables is discussed in the appropriate sections.

Some charts are given for illustrative purposes. In keeping with the general policy of the Editorial Commission, no attempt has been made to make them suitable for direct use. Tables are given for the construction of charts. Many such charts may now be purchased, and information about those currently available can be obtained through some National Committees or Associations. A separate card gives a Table of Proportional Parts.

1.3. Acknowledgments, etc.

The General Editor acknowledges indebtedness to the various authors who have contributed to this Volume, and to proof-readers. Many others have helped in ways too varied to enumerate; some, but not all, have received mention at various stages in the Volume. The staff of The Kynoch Press have taken the greatest possible trouble to see that this volume is as well produced as was Volume I and are in no way responsible for the time that has elapsed between the publication of the two volumes.

In general, notification of numerical or other errors should be made to the General Editor, although in case of doubt direct contact with the author concerned may be more helpful.

Section 2

FUNDAMENTAL MATHEMATICS

A. L. PATTERSON

	PAGE
2.0. INTRODUCTION	5
2.1. ALGEBRA	6
2.2. TRIGONOMETRY AND GEOMETRY	36
2.3. DIFFERENTIAL AND INTEGRAL CALCULUS	50
2.4. VECTOR AND TENSOR ANALYSIS	52
2.5. FOURIER THEORY	65
2.6. STATISTICS (D. W. J. CRUICKSHANK)	84

2.0. Introduction

The purpose of the present chapter is to provide a summary of the mathematical techniques which have been applied to problems of physics and of crystallography of interest in X-ray crystal structure analysis.

Some of the formulae included are elementary and are included because the human memory is very treacherous as to signs and factors in the results of elementary algebra and trigonometry. In the more sophisticated sections no attempt is made to give proofs, but the results are presented in a more or less logical sequence to give them some continuity. The amount of detail provided is intended to be sufficient to recall the main features of a discipline to those who have at some time been exposed to it. While this chapter is not intended to replace a series of mathematical textbooks, it may be of service in indicating to the investigator that a particular discipline unfamiliar to him may have application to the problems on which he is engaged.

A bibliography will be found at the end of the section. An attempt has been made to include references in the bibliography to texts in languages other than that of the writer, but this has been difficult. It is hoped

that those which have been included have sufficient international importance to be available in many libraries. References to the bibliography are given in the text in square brackets, e.g. [14].

Examples are given in many places to indicate the application of a given discipline to crystal-analytical problems. Clearly such indication can only be very incomplete. It is supplemented wherever possible by references to examples of applications from the literature. In these cases no attempt has been made towards completeness, and apology is made in advance to those authors who feel that their paper would have made the ideal example for the application of a particular technique.

Detailed acknowledgment of sources for such a compilation is almost impossible. Many tabulations are classical and have been handed down through generations of texts. Each compiler attempts to take the best of his predecessor's work and to add improvements of his own, it is hoped without the introduction of errors. Almost all the references given have contributed to the present text, some a great deal and others only a little, and this help is very gratefully acknowledged.

2.1. Algebra

2.1.1. Complex Numbers

Definitions

The quantity $z=x+iy$ is a *complex number* if i is the positive root of the equation $i^2=-1$ and x and y are real numbers called respectively the *real part* and the *imaginary part* of z . The complex number $\tilde{z}=x-iy$ is called the *conjugate* of z .

Any complex number can be expressed in any of the forms:

$$z=x+iy=|z|(\cos \phi+i \sin \phi)=|z|e^{i\phi} \quad \dots(1)$$

Here $|z|=(x^2+y^2)^{\frac{1}{2}}=(z\tilde{z})^{\frac{1}{2}}$ is called the *absolute value* (or *magnitude*) of the complex number z and is always taken as positive. The angle ϕ is called the *phase* of z and is the solution of the pair of equations

$$\cos \phi=x/|z| \quad \sin \phi=y/|z| \quad \dots(2)$$

If any angle ϕ satisfies these equations, the angle $\phi+2k\pi$ (k integral) will also satisfy them. The value of $(\phi+2k\pi)$ which lies in the range $0 \leq (\phi+2k\pi) < 2\pi$ is called the *principal value* of ϕ and is usually taken as the solution of (2). It is usual to calculate ϕ as the solution of the single equation

$$\tan \phi=y/x \quad \dots(3)$$

It must be noted that (3) has two roots, ϕ and $\phi+\pi$, in the range 0 to 2π and only one of these is a solution of (2).

The result (1) depends on the series expansions 2.1.2 (13), (14) and (15).

Algebra

The algebra of complex numbers is essentially the same as that of real numbers, with the additional result that in any equation the real part of one side must equal the real part of the other side, and independently the imaginary part of one side must equal the imaginary part of the other side.

A power of a complex number is defined by the equation

$$z^p=|z|^p e^{i(\phi+2k\pi)p} \quad \dots(4)$$

where k is any integer. This is single-valued if the index p is an integer (positive, negative or zero). If p is rational there will be a finite number of values for z^p ; if p is irrational there will be infinitely many such values.

For further discussion see textbooks on the calculus, or on the theory of functions of a complex variable, or any "Cours d'Analyse." See also [1], [2], [8], [12] and [13].

Applications

The applications of complex notation in diffraction theory and in any discipline which involves sinusoidal

waves depend on the fact that complicated trigonometric results have a very simple form in complex notation.

EXAMPLE 1

$$e^{i(A+B)}=e^{iA}e^{iB}$$

corresponds to

$$\begin{aligned} \cos(A+B)+i \sin(A+B) &= (\cos A+i \sin A)(\cos B+i \sin B) \\ &= \cos A \cos B - \sin A \sin B + i(\sin A \cos B + \cos A \sin B) \end{aligned}$$

EXAMPLE 2

$$e^{i3A}=(e^{iA})^3$$

corresponds to

$$\begin{aligned} \cos 3A+i \sin 3A &= \cos^3 A - 3 \cos A \sin^2 A + i(3 \cos^2 A \sin A - \sin^3 A) \\ &= 4 \cos^3 A - 3 \cos A + i(3 \sin A - 4 \sin^3 A) \end{aligned}$$

2.1.2. Series

2.1.2.1. BINOMIAL THEOREM

The series

$$(1+x)^n = 1 + nx + \frac{n(n-1)}{2!}x^2 + \dots + \frac{n!}{r!(n-r)!}x^r + \dots \quad \dots(1)$$

represents one of the values of $(1+x)^n$ whenever it is convergent.

- (a) When n is a positive integer, the series terminates and represents the single value of $(1+x)^n$ for all x .
- (b) If n is any rational number and $-1 < x < 1$, the sum of the series (1) is the real positive value of $(1+x)^n$.
- (c) If n is any number and x is complex $0 \leq |x| < 1$, the series (1) converges to that value of $(1+x)^n$ which tends to 1 when x tends to zero.

Special Cases

$$(1+x)^{-1} = 1 - x + x^2 - x^3 + \dots |x| < 1 \quad \dots(2)$$

$$(1+x)^{\frac{1}{2}} = 1 + \frac{1}{2}x - \frac{1.1}{2.4}x^2 + \frac{1.1.3}{2.4.6}x^3 - \frac{1.1.3.5}{2.4.6.8}x^4 + \dots |x| < 1 \quad \dots(3)$$

$$(1+x)^{-\frac{1}{2}} = 1 - \frac{1}{2}x + \frac{1.3}{2.4}x^2 - \frac{1.3.5}{2.4.6}x^3 + \frac{1.3.5.7}{2.4.6.8}x^4 + \dots |x| < 1 \quad \dots(4)$$

For additional special cases see [6], [7], [9] and [14].

2.1.2.2. MULTINOMIAL THEOREM

If n is a positive integer

$$(a_1+a_2+a_3+\dots+a_s)^n = \sum \binom{n}{r_1 r_2 \dots r_s} a_1^{r_1} a_2^{r_2} \dots a_s^{r_s} \quad \dots(5)$$

where the summation is to be taken over all positive integral or zero values of r_1, r_2, \dots, r_s which satisfy the relation $r_1 + r_2 + r_3 + \dots + r_s = n$

and where $\binom{n}{r_1 r_2 \dots r_s} = \frac{n!}{r_1! r_2! \dots r_s!}$ is a multinomial coefficient.

2.1.2.3. PROGRESSIONS

Arithmetic Progression

$$a + (a+d) + (a+2d) + \dots + [a + (n-1)d] = \frac{1}{2}n[2a + (n-1)d] \quad \dots (6)$$

Geometric Progression

$$a + ar + ar^2 + \dots + ar^{n-1} = a(1-r^n)/(1-r) \quad \dots (7)$$

Powers of Natural Numbers

$$1 + 2 + 3 + \dots + n = \frac{1}{2}n(n+1) \quad \dots (8)$$

$$1^2 + 2^2 + 3^2 + \dots + n^2 = \frac{1}{6}n(n+1)(2n+1) \quad \dots (9)$$

$$1^3 + 2^3 + 3^3 + \dots + n^3 = \frac{1}{4}n^2(n+1)^2 \quad \dots (10)$$

$$1^4 + 2^4 + 3^4 + \dots + n^4 = \frac{1}{30}n(n+1)(2n+1)(3n^2+3n-1) \quad \dots (11)$$

$$1^5 + 2^5 + 3^5 + \dots + n^5 = \frac{1}{12}n^2(n+1)^2(2n^2+2n-1) \quad \dots (12)$$

The series $\sum_{s=1}^n s^{-r}$ cannot be summed in closed form. For discussion of these series see [14] and [16].

2.1.2.4. MISCELLANEOUS POWER SERIES

$$e^x = 1 + x + x^2/2! + x^3/3! + \dots \quad |x| < \infty \quad \dots (13)$$

$$\cos x = 1 - x^2/2! + x^4/4! - x^6/6! + \dots \quad |x| < \infty \quad \dots (14)$$

$$\sin x = x - x^3/3! + x^5/5! - x^7/7! + \dots \quad |x| < \infty \quad \dots (15)$$

$$\tan x = x + x^3/3 + 2x^5/15 + 17x^7/315 + \dots \quad |x| < \pi/2 \quad \dots (16)$$

$$\cosh x = 1 + x^2/2! + x^4/4! + x^6/6! + \dots \quad |x| < \infty \quad \dots (17)$$

$$\sinh x = x + x^3/3! + x^5/5! + x^7/7! + \dots \quad |x| < \infty \quad \dots (18)$$

$$\ln(1+x) = x - \frac{1}{2}x^2 + \frac{1}{3}x^3 - \frac{1}{4}x^4 + \dots \quad |x| < 1 \quad \dots (19)$$

$$\ln\left(\frac{1+x}{1-x}\right) = 2\left[x + \frac{1}{3}x^3 + \frac{1}{5}x^5 + \frac{1}{7}x^7 + \dots\right] \quad |x| < 1 \quad \dots (20)$$

Excellent compilations of useful series are contained in [3], [6], [8], [9], [14], etc.

2.1.3. Mathematical Constants

π	=	3.14159 26536
π^2	=	9.86960 44011
$1/\pi$	=	0.31830 98862
$\sqrt{\pi}$	=	1.77245 38509
e	=	2.71828 18285
$1/e$	=	0.36787 94412
$\log e$	=	0.43429 44819
$\ln 10$	=	2.30258 50930
$\sqrt{2}$	=	1.41421 35624
$\sqrt{3}$	=	1.73205 08076
$\sqrt{5}$	=	2.23606 79775
$\sqrt{7}$	=	2.64575 13111
$\sqrt{10}$	=	3.16227 76602
1 radian	=	57.29577 95131° = 57° 17' 45''
1°	=	0.01745 32925 radian
1'	=	0.00029 08882 radian
1''	=	0.00000 48481 radian

NOTE. log means logarithm to the base 10

ln means logarithm to the base e .

2.1.4. Linear and Rational Independence

Definitions

A set of quantities f_1, f_2, \dots, f_n is said to be *linearly independent* if there exists no relation of the type

$$a_1 f_1 + a_2 f_2 + \dots + a_n f_n = 0 \quad \dots (1)$$

in which the a_i are any constant quantities, real, imaginary or zero, but not all zero.

If the quantities f_i are real numbers, there exist no linearly independent sets. If the quantities f_i are complex numbers or vectors in two-space, there exist infinitely many linearly independent sets of two such quantities. If the quantities f_i are vectors in n -space, there exist infinitely many linearly independent sets of n such quantities. If the quantities f_i are functions of one or more independent variables, there may exist sets of infinitely many linearly independent functions.

A set of quantities f_1, f_2, \dots, f_n are said to be *rationally independent* if there exists no relation of the type (1) in which the a_i are integers, positive, negative or zero, but not all zero.

There exist infinitely many sets of rationally independent real numbers, and, *a fortiori*, the same is true for complex numbers, n -vectors, functions, etc.

Any set of quantities which is linearly independent is of necessity rationally independent.

2.1.5. Modular Algebra (Algebra of Congruences)

When two quantities a and b satisfy the relation

$$a - b = p_1 m_1 + p_2 m_2 + \dots + p_n m_n \quad \dots (1)$$

where p_1, p_2, \dots, p_n are any integers, positive, negative or zero, and m_1, m_2, \dots, m_n is any set of rationally independent quantities, a and b are said to be *congruent*

with respect to the *modulus* (or *modular set*) m_i .† This relation is usually written

$$a \equiv b \pmod{m_i} \quad \dots (2)$$

and is read “ a is congruent to b modulo m_i .”

The algebra of modular congruences is the same as that of equalities except that division of the two sides of the congruence is not always permitted. Division can always be carried out by expressing a congruence such as (2) as an equation such as (1) with arbitrary

$$\text{coefficients } p_i, \text{ i.e. } \frac{a-b}{c} = p_1 \frac{m_1}{c} + p_2 \frac{m_2}{c} + \dots + p_n \frac{m_n}{c}.$$

For further details see any textbook of higher algebra, such as [15] and [16].

The procedure for the solution of a general system of linear congruences with rational coefficients is given in Section 2.1.9.4 (p. 19).

2.1.6. Simple Continued Fractions

A *simple continued fraction* (s.c.f.)‡ is an expression of the form

$$F = q_1 + \frac{1}{q_2 + \frac{1}{q_3 + \frac{1}{q_4 + \dots}}} \quad \dots (1)$$

in which the *quotients* q_i are positive integers and identical with the quotients of the Euclidean algorithm (Table 2.1.6A). If q_1 is zero, the s.c.f. is termed *proper*; if not, *improper*. A convenient abbreviation for (1) is

$$F = q_1 + \frac{1}{q_2 +} \frac{1}{q_3 +} \frac{1}{q_4 +} \dots \quad \dots (2)$$

Any positive real number can be expressed as an s.c.f. An irrational number has infinitely many quotients q_i . A rational number has only a finite number n of

quotients and the s.c.f. terminates. The rational fraction r_i/s_i formed by terminating the s.c.f. at the i th quotient is called the i th convergent of the s.c.f. The n th convergent is thus the value of the continued fraction in the case in which it is rational.

The procedure for the expansion of a rational number a_1/a_2 in an s.c.f. is identical with that of determining the greatest common divisor (g.c.d.) of the numerator a_1 and the denominator a_2 by the Euclidean algorithm. This process is illustrated in column 1 of Table 2.1.6A, and the quotients q_i of the s.c.f. (2) are the quotients of the Euclidean algorithm. The process ends with q_n , which is the first quotient to have a remainder zero. The coefficient of q_n , i.e. a_{n+1} , is the g.c.d. of a_1 and a_2 , and is unity if the fraction a_1/a_2 is in its lowest terms, that is if a_1 and a_2 are relatively prime.

The i th convergent, given by r_i/s_i , is computed from the iterated equations

$$\begin{aligned} r_i &= q_i r_{i-1} + r_{i-2} \\ s_i &= q_i s_{i-1} + s_{i-2} \end{aligned} \quad \dots (3)$$

for $i \geq 2$, with the initial values $r_0=1$, $s_0=0$; $r_1=q_1$, $s_1=1$. The computation scheme is exhibited in the last columns of Table 2.1.6A. The same routine applies to both r and s . The value in one row is obtained by multiplying the q of that row by the value in the preceding row and adding the value in the second preceding row.

Any convenient scheme for the computation of g.c.d. can be substituted for that of column 1 of these tables. Note that if a_1/a_2 is a proper fraction ($a_2 > a_1$) the first step may be omitted if $r_1=0$ is substituted in

† In terms of modular algebra, two points in different cells which are crystallographically equivalent with respect to the lattice are congruent with respect to a primitive triplet of translations of the lattice as modulus.

‡ We are not concerned in this volume with more general forms of continued fractions. See for example [15] and [16].

TABLE 2.1.6A
Computation Scheme for Expansion of a_1/a_2 as a Simple Continued Fraction

$$a_1/a_2 = q_1 + \frac{1}{q_2 +} \frac{1}{q_3 +} \dots \frac{1}{q_n}$$

	i	q_i		
$a_1 = a_2 q_1 + a_3$	0		$r_0 = 1$	$s_0 = 0$
$a_2 = a_3 q_2 + a_4$	1	q_1	$r_1 = q_1$	$s_1 = 1$
	2	q_2	$r_2 = q_2 r_1 + r_0$	$s_2 = q_2 s_1 + s_0$
$a_i = a_{i+1} q_i + a_{i+2}$	i	q_i	$r_i = q_i r_{i-1} + r_{i-2}$	$s_i = q_i s_{i-1} + s_{i-2}$
$a_{n-1} = a_n q_{n-1} + a_{n+1}$	$n-1$	q_{n-1}	$r_{n-1} = q_{n-1} r_{n-2} + r_{n-3}$	$s_{n-1} = q_{n-1} s_{n-2} + s_{n-3}$
$a_n = a_{n+1} q_n + 0$	n	q_n	$r_n = q_n r_{n-1} + r_{n-2}$	$s_n = q_n s_{n-1} + s_{n-2}$

the table. Two numerical examples are given in Table 2.1.6B.

Exactly the same process may be used to expand irrational fractions as continued fractions and to obtain approximations for such irrational fractions by rational fractions, for example the fractions 3, 22/7, 333/106, 355/113, etc., as approximations for π . See [15] and [16] for further discussion.

TABLE 2.1.6B

Expansions in Simple Continued Fractions

EXAMPLE 1. $a_1/a_2=323/221$

	i	q_i	r_i	s_i
	0	—	1	0
$323=221.1+102$	1	1	1	1
$221=102.2+17$	2	2	3	2
$102=17.6$	3	6	19	13

$$323/221=19/13=1+\frac{1}{2+\frac{1}{6}} \quad \text{g.c.d.}=17$$

Convergents: 1, 3/2, (16/11), 19/13

$$323 \times 2 - 221 \times 3 = 646 - 663 = (-1)^3 \times 17$$

$$323 \times 11 - 221 \times 16 = 3553 - 3536 = (-1)^4 \times 17$$

EXAMPLE 2. $a_1/a_2=10/47$

	i	q_i	r_i	s_i
	0	—	1	0
$10=47.0+10$	1	0	0	1
$47=10.4+7$	2	4	1	4
$10=7.1+3$	3	1	1	5
$7=3.2+1$	4	2	3	14
$3=1.3$	5	3	10	47

$$10/47=0+\frac{1}{4+\frac{1}{1+\frac{1}{2+\frac{1}{3}}}} \quad \text{g.c.d.}=1$$

Convergents: 0, 1/4, 1/5, 3/14, (7/33), 10/47

$$10.14 - 47.3 = 140 - 141 = (-1)^5$$

$$10.33 - 47.7 = 330 - 329 = (-1)^6$$

Properties of the Convergents

The first convergent is always less than the value of the s.c.f. and each successive convergent is alternately above and below this value, and closer to it. The value of the n th convergent of a terminating s.c.f. is of course the value of the original fraction.

The property of convergents of most universal application depends on the result that

$$r_i s_{i-1} - r_{i-1} s_i = (-1)^i \quad \dots (4a)$$

and in particular, if a_1 and a_2 are relatively prime,

$$r_n s_{n-1} - r_{n-1} s_n = a_1 s_{n-1} - r_{n-1} a_2 = (-1)^n \dots (4b)$$

The ratio r_{n-1}/s_{n-1} is called the *penultimate convergent*.

If a_1 and a_2 are not relatively prime, then

$$a_1 s_{n-1} - r_{n-1} a_2 = (-1)^n (\text{g.c.d.}) \dots (4c)$$

It should be noted that an *intermediate convergent* (e.g. those shown in parentheses in Table 2.1.6B)

$$\rho/\sigma = (r_n - r_{n-1})/(s_n - s_{n-1}) \dots (5a)$$

may be constructed so that

$$a_1 \sigma - \rho a_2 = (-1)^{n+1} (\text{g.c.d.}) \dots (5b)$$

EXAMPLES

1. Given a primitive translation of any lattice, to find a primitive cell having this translation as one of its primitive translations.

(a) *Two Dimensions*. Consider the transformation

$$A_1 = q_1 a_1 + q_2 a_2$$

$$A_2 = u_1 a_1 + u_2 a_2$$

and assume that u_1 and u_2 are given relatively prime integers, since A_2 is a primitive translation of the lattice. Then if the new cell is to be primitive we must have the determinant of the transformation

$$q_1 u_2 - q_2 u_1 = 1$$

Solutions of equations of this type are given in Table 2.1.6C. If A_1, A_2 is a solution of this problem ($A_1 + nA_2$), A_2 will also be a solution for n integral.

Numerical Example. Let $u_1=3$, $u_2=5$. Then from the table we must have $q_1=2$, $q_2=3$, i.e. $2.5-3.3=1$, and the general solution will be

$$A_1 = (2+3n)a_1 + (3+5n)a_2$$

$$A_2 = 3a_1 + 5a_2$$

The intermediate convergent 2/3 has been used to obtain a net of the same "hand" as the original. The solution using the penultimate convergent 1/2 is obtained from the above by setting $n=-1$.

(b) *Three Dimensions*. Consider the transformation

$$A_1 = a_3$$

$$A_2 = b_1 a_1 + b_2 a_2$$

$$A_3 = u_1 a_1 + u_2 a_2 + u_3 a_3$$

in which $u_1 u_2 u_3$ are given, and must be relative prime if A_3 is primitive. The general form for three relative prime integers is

$$u_i = d_{ki} d_{ij} e_i$$

in which d_{ij} is the highest common factor of u_i and u_j . Thus the sets d_{ij} and e_i are each within themselves pair-wise relative prime, but e_i may have one factor in common with d_{ij} and another (relative prime to the first) in common with d_{jk} .

Under these conditions one must first find all vectors U which are reciprocal to u with relative prime components satisfying

$$u_1 U_1 + u_2 U_2 + u_3 U_3 = 1$$

The general solution for this equation can be expressed as

$$U_i = r_{ki}(q_k - u_k g_k) + d_{jk} e_j h_k$$

$$U_j = r_{kj}(q_k - u_k g_k) - d_{ki} e_i h_k$$

$$U_k = p_k + d_{ij} g_k$$

2.1. ALGEBRA

In these expressions g_k, h_k are arbitrary integers (positive or negative) or zero. The relative prime pair of integers p_k, q_k are a solution of the equation

$$p_k u_k + q_k d_{ij} = 1$$

and the relative prime pair of integers r_{ki}, r_{kj} are a solution of the equation

$$r_{ki} u_i + r_{kj} u_j = d_{ij}$$

There are three representations of the same set of vectors \mathbf{U} which may be obtained by cyclic permutation of the subscripts in the above expressions.

In the second stage of the calculation one must obtain sets of two vectors

$$\mathbf{A}_1 = a_{11}\mathbf{a}_1 + a_{21}\mathbf{a}_2 + a_{31}\mathbf{a}_3$$

$$\mathbf{A}_2 = a_{12}\mathbf{a}_1 + a_{22}\mathbf{a}_2 + a_{32}\mathbf{a}_3$$

(with relative prime components a_{i1}, a_{i2}) whose vector product generates the vector \mathbf{U} . Since the components U_i of this vector are relative prime, they have the same general form as the u_i , i.e.

$$U_i = D_{ki} D_{ij} E_i$$

A particular solution is

$$\mathbf{A}'_1 = m_{ki} D_{jk} E_k \mathbf{a}_i + m_{kj} D_{ki} E_k \mathbf{a}_j - D_{ij} \mathbf{a}_k$$

$$\mathbf{A}'_2 = D_{jk} E_j \mathbf{a}_j + D_{ki} E_i \mathbf{a}_j$$

in which $m_{ki} E_i + m_{kj} E_j = 1$.

The general solution is then

$$\mathbf{A}_1 = s_1 \mathbf{A}'_1 + t_1 \mathbf{A}'_2$$

$$\mathbf{A}_2 = s_2 \mathbf{A}'_1 + t_2 \mathbf{A}'_2$$

provided that $s_1 t_2 - s_2 t_1 = 1$.

Numerical Example. Let $u_1=2, u_2=6, u_3=9$. The only relative prime pair is 2 and 9. Use of Table 2.1.6C then enables us to write

$$\mathbf{A}_1 = \mathbf{a}_2$$

$$\mathbf{A}_2 = \mathbf{a}_1 + 5\mathbf{a}_3$$

$$\mathbf{A}_3 = 2\mathbf{a}_1 + 6\mathbf{a}_2 + 9\mathbf{a}_3$$

2. An application of continued fractions to the location of the maxima of Fourier series expansions has been made by Hauptman and Karle (*Acta Cryst.*, 6, 469, 1953).

3. Gear ratios to approximate the actual values of sines and cosines used in Fourier synthesis (cf. J. M. Robertson, *Acta Cryst.*, 7, 817, 1954) can be obtained from the expansions of these quantities in s.c.f.'s.

4. See also 2.1.9.4 (p. 19) for the reduction of a system of equations valid in a lattice.

TABLE 2.1.6C

Table of Penultimate and Intermediate Convergents for the Ratios a_1/a_2 ($0 < a_1 < a_2 \leq 20$)

Each line of an entry exhibits x_1, x_2 , a solution of one of the equations $a_1 x_2 - a_2 x_1 = \pm 1$

a_1	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
1	0 1 1 0	0 1 1 1	0 1 1 2	0 1 1 3	0 1 1 4	0 1 1 5	0 1 1 6	0 1 1 7	0 1 1 8	0 1 1 9	0 1 1 10	0 1 1 11	0 1 1 12	0 1 1 13	0 1 1 14	0 1 1 15	0 1 1 16	0 1 1 17	0 1 1 18	0 1 1 19
2			1 1 1 2		1 2 1 3		1 3 1 4		1 4 1 5		1 5 1 6		1 6 1 7		1 7 1 8		1 8 1 9		1 9 1 10	
3				1 1 2 3	1 2 2 3		1 2 2 5	1 3 2 5		1 3 2 7	1 4 2 7		1 4 2 9	1 5 2 9		1 5 2 11	1 6 2 11		1 6 2 13	1 7 2 13
4					1 1 3 4		1 2 3 5		1 2 3 7		1 3 3 8		1 3 3 10		1 4 3 11		1 4 3 13		1 5 3 14	
5						1 1 4 5	2 3 3 4	2 3 3 5	1 2 4 7		1 2 4 9	2 5 3 7	2 5 3 8	1 3 4 11		1 3 4 13	2 7 3 10	2 7 3 11	1 4 4 15	
6							1 1 5 6				1 2 5 9		1 2 5 11				1 3 5 14		1 3 5 16	
7								1 1 6 7	3 4 4 5	2 3 5 7	2 3 5 8	3 5 4 7	1 2 6 11		1 2 6 13	3 7 4 9	2 5 5 12	2 5 5 13	3 8 4 11	1 3 6 17
8									1 1 7 8		3 4 5 7		3 5 5 8		1 2 7 13		1 2 7 15		3 7 5 12	
9										1 1 8 9	4 5 5 6		2 3 7 10	2 3 7 11		4 7 5 9	1 2 8 15		1 2 8 17	4 9 5 11
10											1 1 9 10		3 4 7 9				3 5 7 12		1 2 9 17	
11												1 1 10 11	5 6 6 7	4 5 7 9	3 4 8 11	2 3 9 13	2 3 9 14	3 5 8 13	4 7 7 12	5 9 6 11
12													1 1 11 12				5 7 7 10		5 8 7 11	
13														1 1 12 13	6 7 7 8	4 5 9 11	3 4 10 13	5 7 8 11	2 3 11 16	2 3 11 17
14															1 1 13 14		5 6 9 11		3 4 11 15	
15																1 1 14 15	7 8 8 9		4 5 11 14	
16																	1 1 15 16		5 6 11 13	
17																		1 1 16 17	8 9 9 10	6 7 11 13
18																			1 1 17 18	
19																				1 1 18 19

2.1.7. Determinants

The *determinant* which is written

$$\begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix}$$

is by definition equal to $a_{11}a_{22} - a_{12}a_{21}$. This definition is generalized for a determinant of the n th order (i.e. having n rows and n columns) as follows:

$$|a_{ij}| = \begin{vmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{vmatrix} = \sum (\pm) (a_{i_1} a_{j_2} a_{k_3} \dots a_{qn}) \dots (1)$$

where the sequence of numbers i, j, k, \dots, q is a derangement of the n numbers $1, 2, 3, \dots, n$. The sum is taken over all such derangements ($n!$), and the sign of any term is positive if the derangement is even and negative if the derangement is odd. The parity of the derangement is that of the number of interchanges of adjacent numbers required to produce the given derangement from the standard order. Thus 1234, 3124, 4321, etc., are even derangements for $n=4$, and 1243, 2413, 2341, etc., are odd derangements.

The determinant of $(n-1)$ order obtained by deleting the row and column which intersect in a_{ij} (i th row and j th column) is called the *minor* (first minor) m_{ij} of a_{ij} . The *cofactor* A_{ij} of a_{ij} is then defined as

$$A_{ij} = (-1)^{i+j} m_{ij}$$

A determinant of order $(n-s)$ obtained by deleting s rows and s columns is called an *sth minor*. If the deleted rows and columns have corresponding numbers, it is called a *symmetrical sth minor*.

The following are useful properties of determinants:

1. A determinant may be expanded in terms of the members of a column and their cofactors or of the members of a row and their cofactors: i.e.

$$|a_{ij}| = \sum_l a_{lm} A_{lm} = \sum_m a_{lm} A_{lm}$$

2. The value of a determinant is unchanged if rows are taken as columns and columns as rows.
3. Interchange of two rows or of two columns changes the sign of the determinant.
4. Multiplication of all the terms of a single row or a single column by the same number multiplies the determinant by that number.
5. The value of a determinant is unchanged by adding to any one of its rows or columns any linear combination of its other rows or columns.

Application of these rules leads to methods for the evaluation of determinants (see also 2.1.8.10, p. 15).

Rules for the multiplication of determinants form a special case of those for the multiplication of matrices (see 2.1.8.2).

Reference is made to almost any textbook of advanced algebra, e.g. [15]–[19], particularly [17].

2.1.8. Matrices

2.1.8.1. DEFINITIONS

A system of mn quantities arranged in a rectangular array of m rows and n columns is called a *matrix*.

$$\mathbf{a} = [a_{ij}] = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mn} \end{bmatrix} \dots (1)$$

The *transposed matrix* \mathbf{a}' of \mathbf{a} is the matrix which has rows identical with the columns of \mathbf{a} , and vice versa.

When $m=n$ the matrix is a *square matrix*, and the elements a_{ii} lie in the principal diagonal. The sum of the elements a_{ii} of the principal diagonal is called the *trace* (German: *Spur*) of the matrix \mathbf{a} ($\text{tr } \mathbf{a}$). If all the elements other than a_{ii} are zero, the matrix is a *diagonal matrix*. A *unit matrix* is a diagonal matrix in which all the diagonal elements have the value unity. It is represented by the symbol $\mathbf{1}$.

When $a_{ij} = a_{ji}$ a square matrix is said to be *symmetric*. If $a_{ij} = -a_{ji}$ and $a_{ii} = 0$ a square matrix is said to be *skew symmetric*. To save printing, the *column matrix*, i.e. one which has m rows and one column, is represented by the special notation

$$\begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix} \equiv \{b_1, b_2, \dots, b_m\} \dots (2)$$

while the *row matrix*, one with one row and n columns, can be given the normal notation $[c_1, c_2, \dots, c_n]$.

Two matrices are of the same *order* if they have the same number of rows and the same number of columns.

2.1.8.2. BASIC OPERATIONS

Equality. $\mathbf{A} = \mathbf{B}$ if $A_{ij} = B_{ij}$ and \mathbf{A} and \mathbf{B} are of the same order.

Addition. $\mathbf{C} = \mathbf{A} + \mathbf{B}$ if $C_{ij} = A_{ij} + B_{ij}$ and \mathbf{A} , \mathbf{B} , \mathbf{C} are of the same order.

Subtraction. $\mathbf{C} = \mathbf{A} - \mathbf{B}$ if $C_{ij} = A_{ij} - B_{ij}$ and \mathbf{A} , \mathbf{B} , \mathbf{C} are of the same order.

Scalar Multiplication. If r is a scalar, $r\mathbf{A} = \mathbf{A}r = \mathbf{C}$ if $C_{ij} = rA_{ij}$.

The associative and commutative rules for addition, subtraction and scalar multiplication hold good.

NOTE. A single matrix equation implies $(m \times n)$ scalar equations,

$$\text{thus} \quad \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \end{bmatrix} = \begin{bmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \end{bmatrix}$$

implies the six equations $a_{11} = b_{11}$, $a_{12} = b_{12}$, etc.

Matrix Multiplication. The product $\mathbf{P} = \mathbf{BA}$ of two matrices \mathbf{B} (the *pre-factor*) and \mathbf{A} (the *post-factor*) is the matrix whose elements are

$$P_{ij} = \sum_{r=1}^n B_{ir} A_{rj} \dots (3)$$

NOTE

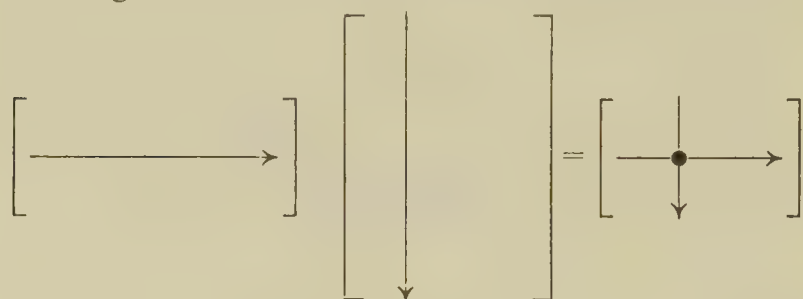
(i) The product can only be formed if the number of columns (n) of the pre-factor is the same as the number of rows of the post-factor.

(ii) The number of rows of the product will be the same as the number of rows of the pre-factor, and the number of columns of the product will be the same as the number of columns of the post-factor.

(iii) The *associative and distributive laws* hold for matrix multiplication. The *commutative law does not necessarily hold*, but two matrices for which $\mathbf{BA}=\mathbf{AB}$ are said to *commute*. The unit matrix $\mathbf{1}$ commutes with any square matrix of the same order.

(iv) In a product of r matrices $\mathbf{P}=\mathbf{A}_r\mathbf{A}_{r-1}, \dots, \mathbf{A}_2\mathbf{A}_1$ the number of columns of the s th matrix must equal the number of rows of the $(s-1)$ th matrix.

(v) A useful mnemonic for matrix multiplication is the diagram



The i th row of the pre-factor multiplied term by term by the j th column of the post-factor is added and entered in the ij position of the product. The following example is illustrative:

$$\begin{bmatrix} 1 & 4 & -2 & 0 \\ 2 & 0 & 1 & 3 \end{bmatrix} \begin{bmatrix} 2 & 5 & 0 \\ 4 & 0 & 0 \\ 1 & 1 & 1 \\ 0 & 1 & 1 \end{bmatrix} = \begin{bmatrix} 16 & 3 & -2 \\ 5 & 14 & 4 \end{bmatrix}$$

2.1.8.3. DETERMINANTS AND RANK

The *determinant* of a square matrix is the determinant whose elements are identical with those of the matrix.

The determinant of the product of two matrices is the product of the determinants of the factors.

A matrix is said to be of *rank* r if it contains at least one square matrix of r rows and columns (either the matrix itself or one obtained from it by deletion of one or more rows and/or columns) whose determinant is non-zero, and no other matrix of higher order whose determinant is non-zero.

A square matrix ($m \times m$) whose rank r is less than m is said to be *singular*. The quantity $(m-r)$ is called the *degeneracy* of the matrix. If r_1 and r_2 are the ranks of two square ($n \times n$) matrices, the rank R_s of the sum satisfies the inequality $R_s \leq r_1 + r_2$. The rank R_p of the product satisfies the three inequalities

$$R_p \leq r_1; R_p \leq r_2; R_p \geq r_1 + r_2 - n$$

If a square ($n \times n$) matrix of rank r is multiplied in either order by a non-singular ($n \times n$) matrix, the product is also of rank r .

2.1.8.4. RECIPROCAL MATRICES

The adjoint $\mathbf{A}=[A_{ji}]$ of the square matrix $\mathbf{a}=[a_{ij}]$ is the matrix whose elements are the transposed cofactors of the element a_{ij} in the determinant $|a_{ij}|$. It then follows that

$$[a_{ij}][A_{ji}]=|a|\mathbf{1} \quad \dots (4a)$$

$$\text{and that} \quad |A_{ji}|=|a|^{n-1} \quad \dots (4b)$$

If the matrix \mathbf{a} is a non-singular square matrix, the elements of the adjoint \mathbf{A} may each be divided by $|a|$. The matrix so obtained is called the *inverse* \mathbf{a}^{-1} of \mathbf{a} , and it follows that

$$\mathbf{a}\mathbf{a}^{-1}=\mathbf{1} \quad \dots (5)$$

From (4a) it is clear that the determinant of any matrix can be obtained by multiplying any row of the matrix by the corresponding column of the adjoint matrix.

A matrix \mathbf{a} whose transposed matrix \mathbf{a}' is equal to its reciprocal \mathbf{a}^{-1} is said to be *orthogonal*. Its determinant has the value $|a|=\pm 1$. If the conjugate complex $\tilde{\mathbf{a}}$ of a matrix \mathbf{a} is equal to its transposed matrix \mathbf{a}' , the matrix is said to be *Hermitian*. Thus a real symmetric matrix is Hermitian.

If the conjugate complex of the transposed matrix (i.e. $\tilde{\mathbf{a}}'$) is equal to the inverse of the original matrix, it is said to be *unitary* and the determinant $|a|=\pm 1$. Real unitary matrices are also orthogonal, and vice versa.

2.1.8.5. CHARACTERISTIC VALUES

Consider the matrix equation

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} u_{11} & u_{12} & \dots & u_{1n} \\ u_{21} & u_{22} & \dots & u_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ u_{n1} & u_{n2} & \dots & u_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \quad \dots (6a)$$

$$\text{i.e. } \mathbf{y}=\mathbf{u}\mathbf{x} \quad \dots (6b)$$

in which the column matrix \mathbf{x} is premultiplied by the square matrix \mathbf{u} to give the column matrix \mathbf{y} . In other words, the set of n variables x_i has been transformed into the set of n variables y_i . (For examples see Vol. I, Sec. 2.5; and Secs. 2.1.6, 2.2.4, 2.2.5 and 2.4 of the present volume.)

It is often necessary to find the *principal axes* of the matrix \mathbf{u} . These axes are also called the *characteristic vectors*[†] of the matrix \mathbf{u} and are represented by the column matrices $\boldsymbol{\xi}$ (see 2.1.8.1), for which

$$\lambda\boldsymbol{\xi}=\mathbf{u}\boldsymbol{\xi} \quad \dots (7)$$

We construct the *characteristic matrix* of \mathbf{u} , i.e.

$$\mathbf{f}(\lambda)=\lambda\mathbf{1}-\mathbf{u} \quad \dots (8)$$

and notice that (7) is equivalent to

$$\mathbf{f}(\lambda)\boldsymbol{\xi}=\mathbf{0} \quad \dots (9)$$

[†] The terms "characteristic function" and "characteristic vectors," due to Hamilton, were translated into German as *Eigenfunktionen* and *Eigenvektoren*. They were then returned to English as *eigenfunctions* and *eigenvectors*.

The condition that a non-zero solution of (9) exists (2.1.9.1, p. 16) is that

$$\Delta(\lambda) = |f(\lambda)| = |\lambda \mathbf{1} - \mathbf{u}| = 0 \quad \dots (10)$$

The determinant $\Delta(\lambda)$ is called the *characteristic determinant*, and the above equation is called the *characteristic equation* for the matrix \mathbf{u} .

The n roots $(\lambda_1, \lambda_2, \dots, \lambda_n)$ of this equation (which may or may not be distinct) are called the *characteristic numbers* of \mathbf{u} .

If λ_i is a simple root of (10), we construct the matrix $\mathbf{F}(\lambda_i)$, which is the adjoint matrix of $\mathbf{f}(\lambda_i)$. This matrix can be resolved into the product of a column matrix and a row matrix, i.e.

$$\mathbf{F}(\lambda_i) = \{\xi_{1i} \xi_{2i} \dots \xi_{ni}\} [\kappa_{i1} \kappa_{i2} \dots \kappa_{in}] \quad \dots (11)$$

If λ_s is one of s multiple roots, and $\mathbf{f}(\lambda_s)$ has degeneracy exactly s , we form the $(s-1)$ st derivative (2.1.8.8) of $\mathbf{F}(\lambda)$ and hence $\mathbf{F}^{s-1}(\lambda_s)$. This can be factored in terms of $(n \times s)$ column and row matrices as follows:

$$\mathbf{F}^{s-1}(\lambda_s) = \begin{bmatrix} \xi_{1,p} & \xi_{1,p+1} & \dots & \xi_{1,p+s-1} \\ \xi_{2,p} & \xi_{2,p+1} & \dots & \xi_{2,p+s-1} \\ \vdots & \vdots & \ddots & \vdots \\ \xi_{n,p} & \xi_{n,p+1} & \dots & \xi_{n,p+s-1} \end{bmatrix} \begin{bmatrix} \kappa_{p,1} & \kappa_{p,2} & \dots & \kappa_{p,n} \\ \kappa_{p+1,1} & \kappa_{p+1,2} & \dots & \kappa_{p+1,n} \\ \vdots & \vdots & \ddots & \vdots \\ \kappa_{p+s-1,1} & \kappa_{p+s-1,2} & \dots & \kappa_{p+s-1,n} \end{bmatrix} \quad \dots (12)$$

If λ_s is one of s multiple roots and the degeneracy of $\mathbf{f}(\lambda_s)$ is $q < s$, only q linearly independent ξ columns can be obtained. If $q=1$ there is only one ξ column, and it is obtained by factoring $\mathbf{F}(\lambda_s)$ as in (11). If $q>1$, the q linearly independent ξ columns must be obtained from the derivatives of $\mathbf{F}(\lambda)$ which are not null when λ_s is substituted. For details see [18].

In those cases in which n column matrices ξ_{si} can be obtained we can construct any one of a number of matrices \mathbf{k} in which the column k_{si} is proportional to the column matrix ξ_{si} . These matrices are non-singular and have the property that

$$\mathbf{u} = \mathbf{k} \mathbf{\Lambda} \mathbf{k}^{-1} \quad \dots (13a)$$

and hence that

$$\mathbf{\Lambda} = \mathbf{k}^{-1} \mathbf{u} \mathbf{k} \quad \dots (13b)$$

in which $\mathbf{\Lambda}$ is a diagonal matrix, having the characteristic numbers of the matrix \mathbf{u} as terms in the leading diagonal. The reduction of \mathbf{u} to a diagonal form is not possible unless the conditions of the preceding paragraph are satisfied.

If \mathbf{u} is Hermitian or unitary, the reduction to diagonal form is always possible. This is true *a fortiori* for real symmetric matrices or real orthogonal matrices.

If \mathbf{u} is Hermitian the characteristic numbers are real and the characteristic vectors orthogonal.

In the case of degeneracy the characteristic vectors as determined by the foregoing method are orthogonal, but any linear combination of the characteristic vectors belonging to the same multiple root is also a characteristic vector belonging to that root.

EXAMPLE. Consider the matrix

$$\mathbf{u} = \begin{bmatrix} 1 & 1 & -1 \\ -1 & 3 & -1 \\ -1 & 1 & 1 \end{bmatrix} \quad \mathbf{f}(\lambda) = \begin{bmatrix} \lambda-1 & -1 & 1 \\ 1 & \lambda-3 & 1 \\ 1 & -1 & \lambda-1 \end{bmatrix}$$

$$\mathbf{F}(\lambda) = \begin{bmatrix} (\lambda-2)^2 & (\lambda-2) & -(\lambda-2) \\ -(\lambda-2) & \lambda(\lambda-2) & -(\lambda-2) \\ -(\lambda-2) & (\lambda-2) & (\lambda-2)^2 \end{bmatrix}$$

$$\Delta(\lambda) = (\lambda-1)(\lambda-2)^2$$

The first root, $\lambda_1=1$, is simple. For it

$$\mathbf{F}(1) = \begin{bmatrix} 1 & -1 & 1 \\ 1 & -1 & 1 \\ 1 & -1 & 1 \end{bmatrix} = \{1, 1, 1\} [1, -1, 1] \text{ and } \xi_1 = \{1, 1, 1\}$$

The twofold root $\lambda=2$ leads to the matrix

$$\mathbf{f}(2) = \begin{bmatrix} 1 & -1 & 1 \\ 1 & -1 & 1 \\ 1 & -1 & 1 \end{bmatrix}$$

which has rank 1 and is thus twofold degenerate. We therefore calculate

$$\mathbf{F}'(\lambda) = \begin{bmatrix} 2(\lambda-2) & 1 & -1 \\ -1 & 2(\lambda-1) & -1 \\ -1 & 1 & 2(\lambda-2) \end{bmatrix}$$

$$\text{and } \mathbf{F}'(2) = \begin{bmatrix} 0 & 1 & -1 \\ -1 & 2 & -1 \\ -1 & 1 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 1 & 1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & 1 & -1 \\ -1 & 1 & 0 \end{bmatrix}$$

and $\xi_2 = \{1, 1, 0\}$, $\xi_3 = \{0, 1, 1\}$ are solutions, and we have

$$\mathbf{k} \mathbf{\Lambda} \mathbf{k}^{-1} = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 1 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{bmatrix} \begin{bmatrix} 1 & -1 & 1 \\ 0 & 1 & -1 \\ -1 & 1 & 0 \end{bmatrix}$$

$$= \mathbf{k} \begin{bmatrix} 1 & -1 & 1 \\ 0 & 2 & -2 \\ -2 & 2 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 1 & -1 \\ -1 & 3 & -1 \\ -1 & 1 & 1 \end{bmatrix}$$

We note also that we may choose instead of ξ_2, ξ_3 any other pair ξ'_2, ξ'_3 such that $\{\xi'_2, \xi'_3\} = \mathbf{M} \{\xi_2, \xi_3\}$ where \mathbf{M} is any non-singular (2×2) matrix.

2.1.8.6. DIAGONALIZATION OF A QUADRATIC FORM

The matrix expression

$$\mathbf{x}' \mathbf{a} \mathbf{x} = [x_i] [a_{ij}] \{x_j\} = \sum_{i=1}^n a_{ii} x_i^2 + 2 \sum_{i < j}^n a_{ij} x_i x_j \quad \dots (14)$$

is known as a *quadratic form*. The matrix \mathbf{a} can be taken as symmetric without loss of generality. In many geometrical and physical problems it is desirable to replace the variables x_i with y_i by means of an orthogonal unitary transformation in such a manner that the new quadratic form has no mixed products $y_i y_j$ and consists only of the squared terms y_i^2 . If we set $\mathbf{x} = \mathbf{q} \mathbf{y}$, then the expression (14) becomes

$$\mathbf{y}' \mathbf{q}' \mathbf{a} \mathbf{q} \mathbf{y} = \mathbf{y}' \mathbf{q}^{-1} \mathbf{a} \mathbf{q} \mathbf{y} = \mathbf{y}' \mathbf{b} \mathbf{y} \quad \dots (15)$$

since $\mathbf{q}' = \mathbf{q}^{-1}$ if \mathbf{q} is an orthogonal unitary transformation. If now the expression is to correspond to a

quadratic form with only squared terms, the matrix $\mathbf{b} = \mathbf{q}^{-1}\mathbf{a}\mathbf{q}$ must be diagonal. Thus the matrix \mathbf{q} must be of the type \mathbf{k} (2.1.8.5 (13)) with the added restriction that the vectors which compose \mathbf{k} must be unitary. Since \mathbf{a} is symmetric, such a reduction is always possible and the characteristic vectors are always orthogonal. The method is illustrated by the following example.

EXAMPLE. Consider the quadratic form

$$2x_1^2 + 2x_2^2 - 4x_3^2 - 2x_1x_2 + 10x_2x_3 + 10x_3x_1$$

We have

$$\Delta(\lambda) = \begin{vmatrix} \lambda-2 & 1 & -5 \\ 1 & \lambda-2 & -5 \\ -5 & -5 & \lambda+4 \end{vmatrix} = \lambda^3 - 63\lambda + 162 = 0$$

The solution of the characteristic equation is often the most difficult part of the operation. In this case, chosen for simplicity, we have

$$\Delta(\lambda) = (\lambda-6)(\lambda-3)(\lambda+9) = 0$$

To find the characteristic vectors, we write

$$\mathbf{F}(\lambda) = \begin{bmatrix} \lambda^2 + 2\lambda - 33 & 21 - \lambda & 5(\lambda - 3) \\ 21 - \lambda & \lambda^2 + 2\lambda - 33 & 5(\lambda - 3) \\ 5(\lambda - 3) & 5(\lambda - 3) & \lambda^2 - 4\lambda + 3 \end{bmatrix}$$

For the first vector we consider

$$\mathbf{F}(6) = \begin{bmatrix} 15 & 15 & 15 \\ 15 & 15 & 15 \\ 15 & 15 & 15 \end{bmatrix} = 15\{111\}[111]$$

Thus the first vector when normalized will be $1/\sqrt{3}$, $1/\sqrt{3}$, $1/\sqrt{3}$. By considering $\mathbf{F}(3)$ we get $-1/\sqrt{2}$, $1/\sqrt{2}$, 0, and from $\mathbf{F}(-9)$ we get $1/\sqrt{6}$, $1/\sqrt{6}$, $-2/\sqrt{6}$ for the remaining vectors. Thus

$$\begin{aligned} \mathbf{b} &= \begin{bmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & -\frac{2}{\sqrt{6}} \end{bmatrix} \begin{bmatrix} 2 & -1 & 5 \\ -1 & 2 & 5 \\ 5 & 5 & -4 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{3}} & 0 & -\frac{2}{\sqrt{6}} \end{bmatrix} \\ &= \begin{bmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & -\frac{2}{\sqrt{6}} \end{bmatrix} \begin{bmatrix} 2\sqrt{3} & -\frac{3}{\sqrt{2}} & -\frac{9}{\sqrt{6}} \\ 2\sqrt{3} & \frac{3}{\sqrt{2}} & -\frac{9}{\sqrt{6}} \\ 2\sqrt{3} & 0 & \frac{18}{\sqrt{6}} \end{bmatrix} \begin{bmatrix} 6 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & -9 \end{bmatrix} \end{aligned}$$

The quadratic form is now

$$6y_1^2 + 3y_2^2 - 9y_3^2 = \lambda_1 y_1^2 + \lambda_2 y_2^2 + \lambda_3 y_3^2$$

and the transformation is

$$\{x_i\} = \begin{bmatrix} \frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{3}} & 0 & -\frac{2}{\sqrt{6}} \end{bmatrix} \{y_i\}$$

2.1.8.7. TRANSFORMATIONS OF MATRICES

Elementary Operations

The *elementary operations* on matrices consist of the following:

- I(a) Interchange of the i th and j th rows.
- (b) Interchange of the i th and j th columns.
- II(a) Addition to the i th row of a multiple of the j th row.
- (b) Addition to the i th column of a multiple of the j th column.
- III(a) Multiplication of the i th row by a non-zero constant.
- (b) Multiplication of the i th column by a non-zero constant.

Operations of type I consist of multiplications by a matrix \mathbf{J} which is derived from the unit matrix by interchange of rows i and j (or of columns i and j). Used as a premultiplier it will interchange rows; as a post-multiplier it will interchange columns.

Operations of type II consist of multiplications by the matrix \mathbf{M} which is derived from the unit matrix by adding the non-zero constant m in the i th row of the j th column. In \mathbf{Mu} then the product is obtained from \mathbf{u} by adding m times the j th row to the i th row. In \mathbf{uM} , m times the i th column is added to the j th column.

Operations of type III consist of multiplications by the matrix \mathbf{H} which is derived from the unit matrix by replacing the i th entry in the diagonal (i th row, i th column) by the non-zero constant h .

The operating matrices are non-singular, so that rank is preserved under elementary operations. The operations \mathbf{J} and \mathbf{M} have unit positive determinants, so that the value of the determinant of the matrix is preserved under operations of types I and II. Operations of type III multiply the value of the determinant by the constant h .

Equivalent Matrices and Canonical Forms

Two matrices are said to be *equivalent* if they can be derived from each other by a finite number of elementary operations. It then follows that, if \mathbf{u} and \mathbf{v} are equivalent,

$$\mathbf{v} = \mathbf{PuQ} \quad \dots (16a)$$

where \mathbf{P} and \mathbf{Q} are any non-singular matrices, and that the rank of \mathbf{v} is the same as that of \mathbf{u} .

Any square matrix of rank r is equivalent to a *canonical* (or standard type) matrix all of whose elements are zero except for r units occupying the r leading positions in the principal diagonal. Such a matrix is more strictly described as "*canonical* under elementary operations" (see 2.1.8.10).

If a square matrix of rank r has integral elements and if the multipliers m and h in the matrices \mathbf{M} and \mathbf{H} are restricted to integral values, it is equivalent to a *canonical* (or standard) matrix all of whose elements are zero except for r diagonal elements $\delta_1, \delta_2, \dots, \delta_r$,

such that δ_{s-1} is a factor of δ_s . Such a matrix is more strictly described as “canonical under integral operations” (see 2.1.9.4 for the technique of this reduction).

If the matrices \mathbf{P} and \mathbf{Q} are reciprocal, the transformation

$$\mathbf{w} = \mathbf{Q}^{-1} \mathbf{u} \mathbf{Q} \quad \dots (16b)$$

is called a *similarity transformation* or a *collineatory transformation*. In 2.1.8.5 the conditions are given under which this type of transformation will reduce a matrix to a diagonal canonical form.

2.1.8.8. DIFFERENTIATION OF MATRICES

If the terms of a matrix are all functions of a single independent variable, the derivative of the matrix with respect to that variable is the matrix whose terms are the derivatives of the terms of the original matrix.

The differentiation of products and of other functions of matrices follows in general the customary rules, except that the order of factors must be preserved and division is only possible if an inverse exists. The following examples illustrate these points:

$$\frac{d}{dt}(\mathbf{u}_1 + \mathbf{u}_2) = \frac{d\mathbf{u}_1}{dt} + \frac{d\mathbf{u}_2}{dt} \quad \dots (17a)$$

$$\frac{d}{dt}(\mathbf{u}_1 \mathbf{u}_2) = \mathbf{u}_1 \frac{d\mathbf{u}_2}{dt} + \frac{d\mathbf{u}_1}{dt} \mathbf{u}_2 \quad \dots (17b)$$

$$\frac{d}{dt}(\mathbf{u}^3) = \frac{d\mathbf{u}}{dt} \mathbf{u}^2 + \mathbf{u} \frac{d\mathbf{u}}{dt} \mathbf{u} + \mathbf{u}^2 \frac{d\mathbf{u}}{dt} \quad \dots (17c)$$

$$\frac{d\mathbf{u}^{-1}}{dt} = -\mathbf{u}^{-1} \frac{d\mathbf{u}}{dt} \mathbf{u}^{-1}, \text{ from } \frac{d(\mathbf{u} \mathbf{u}^{-1})}{dt} = 0 \quad \dots (17d)$$

Since in these tables we shall make only occasional use of the differential calculus of matrices, and no use of the integral calculus of matrices, reference must be made to [18], [19] and [20] for further information on these topics.

2.1.8.9. FUNCTIONS OF A MATRIX

The method for the construction of polynomials of a single matrix follows from the rules of the algebra of matrices, and if the matrix is non-singular such polynomials may include negative integral powers.

In cases in which the matrix \mathbf{u} can be diagonalized (2.1.8.5–6, p. 12) more general functions can be constructed. This process depends on the result that the $\mathbf{\Lambda}$ matrix (13) has the property that

$$\phi(\mathbf{\Lambda}) = \begin{bmatrix} \phi(\lambda_1) & 0 & \dots & 0 \\ 0 & \phi(\lambda_2) & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \phi(\lambda_n) \end{bmatrix} \quad \dots (18)$$

in which $\phi(\lambda_i)$ is a given function of the characteristic number λ_i and $\phi(\mathbf{\Lambda})$ is the same function† of the matrix $\mathbf{\Lambda}$. It may then be shown that

$$\phi(\mathbf{u}) = \mathbf{k} \phi(\mathbf{\Lambda}) \mathbf{k}^{-1} \quad \dots (19)$$

The results of this section are applicable to a large range of function types and to most of the matrices

which are likely to arise in physical or in crystallographic problems. For discussions of the limits of applicability of these results reference is made to [18], [19] and [20].

2.1.8.10. NUMERICAL CALCULATIONS WITH MATRICES

NOTE. The present section is intended only to indicate simple methods which may be used in specific problems in the absence of other reference material. The methods given are not necessarily the most efficient or the most rapid. If many such calculations are to be performed reference should be made to [18], etc. Programmes are also available for machine computations with matrices.

Calculations involving matrices with two or three rows and/or columns, with simple numbers as terms, are best carried out directly. If the number of rows and columns is greater than three, and even in the case of 3×3 matrices, the calculations are best made on a systematic basis as suggested below.

The general philosophy of matrix calculations involves the reduction of the matrix to a simple form before performing any manipulations with it. A record is kept of the operations performed by carrying them out at the same time on the unit matrix.

Reduction of a Matrix

By *reduction* of a matrix we mean the transformation of a matrix to an equivalent form (Section 2.1.8.7) by means of the elementary operations. The purpose of such a transformation is to simplify the form of the matrix so that its rank can immediately be evaluated. If we keep track of the operations which we have performed we can at the same time evaluate the determinant and the inverse of any matrix which is non-singular. If we consider the equation

$$\mathbf{u}^{-1} \mathbf{u} = \mathbf{1} \quad \dots (20)$$

and post-multiply it by a series of elementary operations \mathbf{M}_i (2.1.8.7) we have

$$\mathbf{u}^{-1} (\mathbf{u} \mathbf{M}_1 \mathbf{M}_2 \dots \mathbf{M}_n) = \mathbf{1} (\mathbf{M}_1 \mathbf{M}_2 \dots \mathbf{M}_n) \quad \dots (21)$$

It is then clear that if

$$(\mathbf{u} \mathbf{M}_1 \mathbf{M}_2 \dots \mathbf{M}_n) = \mathbf{1} \quad \dots (22)$$

$$\text{then } \mathbf{u}^{-1} = (\mathbf{M}_1 \mathbf{M}_2 \dots \mathbf{M}_n) \quad \dots (23)$$

Thus if we perform a series of elementary operations by post-multiplication (by rows) on \mathbf{u} until \mathbf{u} is reduced to the unit matrix (22) and at the same time carry out the same post-multiplications on the unit matrix, we evaluate the inverse matrix \mathbf{u}^{-1} . If at the same time we keep track of all the operations of type III (2.1.8.7), that is, of those which alter the value of the determinant of the matrix, we can directly determine the value of the determinant $|\mathbf{u}|$.

† Note, however, that if $\phi(\lambda_i)$ is a multiple-valued function with m values, $\phi(\mathbf{\Lambda})$ is multiple-valued with m^n values. Thus $\sqrt{\lambda_i}$ is 2-valued and $\sqrt{\mathbf{\Lambda}}$ is 2^n -valued.

In Table 2.1.8.10A we reduce a given matrix u (left array) to triangular and then to diagonal form by post-multiplication elementary operations on rows alone. We keep track of the operations which we perform by applying them also to the unit matrix (right array). At stage I we have completed the reduction to a triangular form and have obtained a matrix whose determinant is unity. Thus it follows from 2.1.8.3 (p. 12) that the rank of the original matrix and of all the equivalent matrices under the heading "Left Array" is three. The operator matrix at this stage has a determinant whose value is $1/48$. Thus the determinant of the original matrix has the value 48. Proceeding to stage II, we complete the reduction to the diagonal form. From (23) it is clear that the operator matrix in the "Right Array" column is the inverse of u , i.e. u^{-1} , and from (4a) that the adjoint U of u is $|u|u^{-1}$. The reduction could equally well have been carried out in terms of columns.

TABLE 2.1.8.10A
Reduction of a Non-singular Matrix

Operation	Row No.	Left Array	Right Array	
	(1)	36 16 4	1 0 0	
	(2)	15 9 3	0 1 0	
	(3)	6 4 2	0 0 1	
$\frac{1}{4}(1)$	(4)	9 4 1	$\frac{1}{4}$ 0 0	
$\frac{1}{3}(2)$	(5)	5 3 1	0 $\frac{1}{3}$ 0	
$\frac{1}{2}(3)$	(6)	3 2 1	0 0 $\frac{1}{2}$	
(4)-(6)	(7)	6 2 0	$\frac{1}{4}$ 0 $-\frac{1}{2}$	
(5)-(6)	(8)	2 1 0	0 $\frac{1}{3}$ $-\frac{1}{2}$	
	(6)	3 2 1	0 0 $\frac{1}{2}$	
$\frac{1}{2}(7)-(8)$	(9)	1 0 0	$\frac{1}{8}$ $-\frac{1}{3}$ $\frac{1}{4}$	(I)
	(8)	2 1 0	0 $\frac{1}{3}$ $-\frac{1}{2}$	
	(6)	3 2 1	0 0 $\frac{1}{2}$	
(8)-2(9)	(9)	1 0 0	$\frac{1}{8}$ $-\frac{1}{3}$ $\frac{1}{4}$	
	(10)	0 1 0	$-\frac{1}{4}$ 1 -1	(II)
(6)-3(9)-2(10)	(11)	0 0 1	$\frac{1}{8}$ -1 $\frac{7}{4}$	

Results

$$u = \begin{bmatrix} 36 & 16 & 4 \\ 15 & 9 & 3 \\ 6 & 4 & 2 \end{bmatrix} \quad u^{-1} = \begin{bmatrix} \frac{1}{8} & -\frac{1}{3} & \frac{1}{4} \\ -\frac{1}{4} & 1 & -1 \\ \frac{1}{8} & -1 & \frac{7}{4} \end{bmatrix}$$

$$U = \begin{bmatrix} 6 & -16 & 12 \\ -12 & 48 & -48 \\ 6 & -48 & 84 \end{bmatrix}$$

$$|u| = 48 \quad |u^{-1}| = 1/48 \quad \text{Rank of } u = 3$$

In Table 2.1.8.10B the same routine is applied to a singular matrix whose determinant is of course zero. This routine does not lead to a calculation of the adjoint of a singular matrix. For a 3×3 matrix the adjoint is, of course, easily calculated directly. For matrices of higher order, routines are given in 4.12 of reference [18]. It should be remembered that if the degeneracy of the matrix is greater than unity the adjoint is a null matrix.

For further examples of the application of reduction routines see 2.1.9.

TABLE 2.1.8.10B
Reduction of a Singular Matrix

Operation	Row No.	Left Array	Right Array
	(1)	3 1 -1	1 0 0
	(2)	15 9 3	0 1 0
	(3)	6 4 2	0 0 1
-(1)	(4)	-3 -1 1	-1 0 0
(2)+3(1)	(5)	24 12 0	3 1 0
(3)+2(1)	(6)	12 6 0	2 0 1
(5)/12	(4)	-3 -1 1	-1 0 0
(6)/6	(7)	2 1 0	$\frac{1}{4}$ $\frac{1}{12}$ 0
	(8)	2 1 0	$\frac{1}{3}$ 0 $\frac{1}{6}$
(8)-(7)	(4)	-3 -1 1	-1 0 0
	(7)	2 1 0	$\frac{1}{4}$ $\frac{1}{12}$ 0
	(9)	0 0 0	$\frac{1}{12}$ $-\frac{1}{12}$ $\frac{1}{6}$

Calculation of Characteristic Numbers

In the case of square matrices of order (4×4) or less the best routine for the calculation of the characteristic numbers is perhaps the direct expansion of the determinant $\Delta(\lambda)$ of equation (10); one such example has already been given in 2.1.8.5 (p. 12). If the characteristic vectors are required they can be calculated as indicated in Section 2.1.8.5. For matrices of high order such a simple procedure becomes extremely tedious. Slightly less tedious procedures of a more sophisticated nature are available, and for these reference must be made to [18] and to discussions of quantum mechanical calculations.

2.1.9. Linear Equations

2.1.9.1. NON-HOMOGENEOUS SYSTEMS

Consider the system of m linear equations in n variables:

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + \dots + a_{1n}x_n + b_1 &= 0 \\ a_{21}x_1 + a_{22}x_2 + \dots + a_{2n}x_n + b_2 &= 0 \\ &\vdots \\ a_{m1}x_1 + a_{m2}x_2 + \dots + a_{mn}x_n + b_m &= 0 \end{aligned} \quad \dots (1)$$

The matrix $\mathbf{a} = \begin{bmatrix} a_{11}a_{12} & \dots & a_{1n} \\ a_{21}a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \vdots \\ a_{m1}a_{m2} & \dots & a_{mn} \end{bmatrix}$ is called the *matrix of*

the system, while the matrix $\mathbf{b} = \begin{bmatrix} a_{11}a_{12} & \dots & a_{1n}b_1 \\ a_{21}a_{22} & \dots & a_{2n}b_2 \\ \vdots & \vdots & \vdots \\ a_{m1}a_{m2} & \dots & a_{mn}b_m \end{bmatrix}$

is called the *augmented matrix* of the system.

1. If the rank of the matrix \mathbf{a} is less than the rank of \mathbf{b} , there is no solution and the equations are inconsistent.
2. If the matrix \mathbf{a} and the matrix \mathbf{b} both have the same rank r , and there are n unknowns, the values of $(n-r)$ unknowns may be assigned at pleasure and the r others will then be uniquely determined. The $(n-r)$ unknowns whose values may be assigned at pleasure may be chosen in any way provided that the matrix of the coefficients of the remaining unknowns is of rank r .
3. The solution of a system of rank r ($\leq n$) is obtained by using any one of the available square matrices of rank r contained in \mathbf{a} as the matrix of a system of r equations in the r unknowns associated with the terms of the matrix. Any unused equations are discarded, and the $(n-r)$ unknowns not associated with the terms of the $(r \times r)$ matrix are disposable and are included explicitly with their appropriate coefficients as part of the coefficients b_i . The solution of this system of equations, obtained by the method given below for a system of n equations in n variables, is then a solution of the original system of m equations in n variables.

A non-homogeneous system of n equations in n variables has a unique solution provided that the matrix of the system is of rank n , i.e. the determinant of the system matrix does not vanish. Let the system be written in the form

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + \dots + a_{1n}x_n &= y_1 \\ a_{21}x_1 + a_{22}x_2 + \dots + a_{2n}x_n &= y_2 \\ \vdots & \\ a_{n1}x_1 + a_{n2}x_2 + \dots + a_{nn}x_n &= y_n \end{aligned} \quad \dots(2)$$

Then the solution is uniquely

$$x_1 = a_1/a, x_2 = a_2/a, \dots, x_n = a_n/a \quad \dots(3a)$$

where a is the non-zero determinant

$$a = \begin{vmatrix} a_{11}a_{12} & \dots & a_{1n} \\ a_{21}a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \vdots \\ a_{n1}a_{n2} & \dots & a_{nn} \end{vmatrix} \quad \dots(3b)$$

and a_j is the determinant obtained from a by replacing the j th column by the elements y_1, y_2, \dots, y_n . This solution is complete algebraically, but it probably does not provide the easiest numerical routine (Section 2.1.9.3). The solution of the system of equations (2)

can be written very briefly in matrix notation. If the variables x_i are written in order as the column matrix $\mathbf{x} = \{x_1, x_2, \dots, x_n\}$ and similarly the variables y_i as the column matrix $\mathbf{y} = \{y_1, y_2, \dots, y_n\}$, then (2) takes the abbreviated form

$$\mathbf{ax} = \mathbf{y} \quad \dots(4)$$

and the solution, which is written

$$\mathbf{x} = \mathbf{a}^{-1}\mathbf{y} \quad \dots(5)$$

involves the computation of the matrix \mathbf{a}^{-1} , the inverse of \mathbf{a} .

2.1.9.2. HOMOGENEOUS SYSTEMS

1. If in the equations (1) the terms b_i are all zero, the system (called a *homogeneous system*) always has one or more solutions, since the matrix \mathbf{a} always has the rank of the matrix \mathbf{b} .
2. If the rank of the matrix \mathbf{a} is r , the values of $(n-r)$ of the unknowns may be assigned at pleasure. The others are then uniquely determined.
3. If the rank of the matrix \mathbf{a} is n , the only solution is the trivial solution $x_1 = x_2 = \dots = x_n = 0$.
4. The necessary and sufficient condition for a non-trivial solution is that the rank of the matrix of the system shall be less than n .
5. Thus the necessary and sufficient condition for a non-trivial solution is that the determinant of the matrix of the system shall vanish, i.e. $|\mathbf{a}| = 0$.
6. Any homogeneous system for which a non-trivial solution exists can be reduced to a non-homogeneous system of rank $r < n$ which is soluble by the methods given for non-homogeneous systems. This is done as described above by using any one of the available $(r \times r)$ square matrices as the matrix of a non-homogeneous system. Any unused equations are discarded, and the $(n-r)$ unknowns not associated with the terms of the chosen system matrix are included explicitly as part of the coefficients b_i . The solution is then concluded as that of a non-homogeneous system of r equations in r variables whose system determinant does not vanish.

2.1.9.3. NUMERICAL SOLUTION OF A SYSTEM OF LINEAR EQUATIONS

In order to calculate the solution of the equation

$$\mathbf{ax} = \mathbf{h} \quad \dots(6a)$$

it is possible to calculate \mathbf{a}^{-1} by one of the methods referred to in 2.1.8.10 (page 15) and then to use the solution

$$\mathbf{x} = \mathbf{a}^{-1}\mathbf{h} \quad \dots(6b)$$

If \mathbf{h} is given literally, this is the best procedure. If \mathbf{h} is given numerically, the best procedure is to reduce \mathbf{a} to $\mathbf{1}$ by operating from the left and at the same time to operate directly on the column \mathbf{h} . The routine,

which is closely analogous to that of Tables 2.1.8.10, is exhibited in Table 2.1.9.3A for the case

$$\begin{bmatrix} 1 & 0 & 3 & 1 \\ 4 & -1 & 1 & -2 \\ 1 & 3 & 0 & 5 \\ 3 & -1 & 2 & 1 \\ 1 & 3 & 4 & 9 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 2 \\ 1 \\ -1 \\ 3 \\ 3 \end{bmatrix}$$

TABLE 2.1.9.3A
Solution of Linear Simultaneous Equations
 (see reference [18])
Five equations and four unknowns: Solution
unique non-zero

Operation	Row No.	Left Array	Column
	(1)	1* 0 3 1*	2
	(2)	4 -1 1 -2	1
	(3)	1 3 0 5	-1
	(4)	3 -1 2 1	3
	(5)	1 3 4 9	3
(2)-4(1)	(6)	0 -1 -11 -6	-7
(3)-(1)	(7)	0 3 -3 4	-3
(4)-3(1)	(8)	0 -1* -7 -2*	-3
(5)-(1)	(9)	0 3 1 8	1
(8)-(6)	(10)	0 0 4* 4*	4
3(8)+(7)	(11)	0 0 -24 -2	-12
3(8)+(9)	(12)	0 0 -20 2	-8
6(10)+(11)	(13)	0 0 0 22*	12
5(10)+(12)	(14)	0 0 0 22	12
(14)-(13)	(15)	0 0 0 0*	0
-(8)	(1)	1* 0 3 1	2
(10)/4	(8')	0 1* 7 2	3
(13)/22	(10')	0 0 1* 1	1
	(13')	0 0 0 1**	6/11
	(15)	0 0 0 0	0
(1)-(13')	(16)	1* 0 3 0	16/11
(8')-2(13')	(17)	0 1* 7 0	21/11
(10')-(13')	(18)	0 0 1* 0**	5/11
(16)-3(18)	(19)	1* 0 0 0*	1/11
(17)-7(18)	(20)	0 1* 0 0**	-14/11
	(19)	1 0 0 0	1/11
	(20)	0 1 0 0	-14/11
	(18)	0 0 1 0	5/11
	(13')	0 0 0 1	6/11

Solution: $\{x_1 x_2 x_3 x_4\} = \{1/11, -14/11, 5/11, 6/11\}$

NOTES

* At these stages the choice of row to be used in elimination and retained and of the variable to be eliminated is arbitrary. It may or may not be profitable here to reduce the coefficient of the variable to be eliminated to unity in some or all rows. The starred rows are dropped as they are used and then re-assembled at stage X.

** At these stages only the coefficients used in the previous elimination of variables (and still given a single star for that reason) may now be used (in any order of rows) for the elimination of the other coefficients in the same column. Again the double-starred rows used in the elimination are dropped as they are used and reassembled at the end.

At stage X it is clear that the ranks of the system matrix and of its augmented matrix are both 4 and that a solution therefore exists.

This method of reduction is applicable to any system of linear simultaneous equations, homogeneous or non-homogeneous, without previous investigation of the rank of the determinant of the system or of its augmented system. The nature of the solution is indicated directly by the routine solution. Thus the above system has a unique non-zero solution. An example of a non-homogeneous system in which the variables are under-determined (leading to a solution involving variable parameters) is exhibited in Table 2.1.9.3B, while Table 2.1.9.3C presents a case in which the equations are incompatible. The same routine is of course applicable to homogeneous systems.

TABLE 2.1.9.3B
Solution of Linear Simultaneous Equations
 (see reference [18])
Variables under-determined

Operation	Row No.	Left Array	Column
Note (a)	(1)	2* 2 5 3*	5
	(2)	6 1 5 4	5
	(3)	4 -1 0 1	0
	(4)	2 0 1 1	1
(2)-3(1)	(5)	0 -5* -10 -5*	-10
(3)-2(1)	(6)	0 -5 -10 -5	-10
(4)-(1)	(7)	0 -2 -4 -2	-4
(6)-(5)	(8)	0 0 0 0	0
5(7)-2(5)	(9)	0 0 0 0	0
-(5)/5	(1)	2 2 5 3	5
	(10)	0 1 2 1	2
	(8)	0 0 0 0	0
	(9)	0 0 0 0	0
Note (b)	(11)	2 2 0 0	5-5 α -3 β
	(12)	0 1 0 0	2-2 α - β
	(13)	0 0 1 0	α
	(14)	0 0 0 1	β
$\frac{1}{2}(11)-(12)$	(15)	1 0 0 0	$\frac{1}{2}(1-\alpha-\beta)$
	(12)	0 1 0 0	2-2 α - β
	(13)	0 0 1 0	α
	(14)	0 0 0 1	β

Solution

$$\{x_1 x_2 x_3 x_4\} = \{\frac{1}{2}, 2, 0, 0\} + \alpha\{-\frac{1}{2}, -2, 1, 0\} + \beta\{-\frac{1}{2}, -1, 0, 1\}$$

NOTES

(a) The rows and the variables used in the elimination are starred and are dropped after they have been used. They are reassembled at stage X.

(b) At stage X the presence of the rows with zero coefficients and with zero in the right-hand column entry, indicates undetermined variables, and therefore in the present case any two variables may assume arbitrary values. We have taken $x_3 = \alpha$, $x_4 = \beta$.

(c) The equation system (square matrix) is completed by the assumption of arbitrary values for x_3 , x_4 as above, and the record of this operation is transferred to the column symbol.

TABLE 2.1.9.3C
Solution of Linear Simultaneous Equations
Equations incompatible

Operation	Row No.	Left Array			Column
	(1)	1*	1	-2	4
	(2)	2	3	-1	1
	(3)	1	4	7	3
(2)-2(1)	(4)	0	1*	3	-7
(3)-(1)	(5)	0	3	9	-1
(5)-3(4)	(6)	0	0	0	20
Note (a)					
Note (a)	(1)	1	1	-2	4
	(4)	0	1	3	-7
	(6)	0	0	0	20

NOTE

(a) It is clear here that an equation with zero coefficients cannot equal a non-zero quantity, and that the equations are therefore incompatible.

For simplicity the examples presented have been selected to have integral coefficients in the square and in the column matrices. This is, of course, not necessary, and the methods are well adapted to machine computation. It should be noticed that many steps which have been written out in these schemes for clarity's sake can be omitted by the practised computer.

In these schemes we have reduced the system matrix by operations on rows alone because this is perhaps the simplest. For an example in which the reduction makes use of both rows and columns reference is made to Table 2.1.9.4A.

Accounts of routines for the solution of linear equations which differ in arrangement from those presented here are given in many places, e.g. [24], [25] and [26].

2.1.9.4. SOLUTIONS OF HOMOGENEOUS SYSTEMS VALID IN A LATTICE

In crystallography the equation $5x=0$ has the meaning that x can be one-fifth of any translation of a crystal lattice. Thus $5x=0$ has only one solution ($x=0$) in ordinary algebra, while in modular algebra (2.1.5, p. 7) the set of solutions $x=pm/5$ is valid where m is a modulus and p any integer. Methods for the reduction of systems of linear equations with integral coefficients which are valid under modular algebra depend on the reduction of the matrix of the system to canonical form under unitary integral elementary operations. The operations are therefore of Types I, II and III (2.1.8.7, p. 14) using integral multipliers only, since division is not permitted in the general sense (Section 2.1.5). The reduction to canonical form involves operations on both rows and columns and cannot in general be completed by row operations or column operations alone.

The theoretical background of the reduction process is as follows. If the equation system is of the form

$$ax=0 \quad \dots (7)$$

and the matrix a is subjected to a series of elementary operations from the left, i.e. to manipulations of rows alone, the equation system is equivalent to

$$(\lambda a)x=0 \quad \dots (7a)$$

i.e. an equation system with a new set of coefficients (λa) but the same set of variables. If the elementary operations on the matrix a are applied from the right, the system (7) becomes equivalent to

$$(a\rho)\rho^{-1}x=0 \quad \dots (7b)$$

a system with a new set of coefficients $(a\rho)$ and a new set of variables x' connected with the old set x by the relation

$$x'=\rho^{-1}x \quad \dots (7c)$$

or its equivalent

$$x=\rho x'$$

which may be written

$$x=(1\rho)x' \quad \dots (7d)$$

Thus the result of a succession of row and column operations is the system

$$(\lambda a\rho)x'=0 \quad \dots (7e)$$

in which x' is related to x by (7d).

Appropriate row and column operations are applied to the matrix a to reduce it to the canonical form (Section 2.1.8.7) in which all terms are zero except the diagonal terms. These in succession have the values δ_i such that δ_i is a factor of δ_{i+1} , except that after δ_r (where r is the rank of the matrix a) $\delta_{r+1}=0$.

The reduction of the matrix a and the simultaneous development of the matrix (1ρ) may be followed in the example of Table 2.1.9.4A. In this process all operations on columns (multiplications from the right) are performed both on the matrix a and on the unit matrix. Operations on rows (multiplications from the left) are performed on the system matrix a alone.

The motivation of the reduction scheme depends on the fact that δ_1 , the leading diagonal term of the canonical form, must be the greatest common divisor (g.c.d.) of all the terms of the original matrix. Thus one must exhibit this g.c.d. and move it to the leading position, using only the permitted operations. The steps are as follows:

- (a) If the g.c.d. appears explicitly, it is moved by row column interchanges to the a_{11} position and step 2 follows. (b) If the g.c.d. does not appear explicitly, it must be exhibited by means of the Euclidean algorithm (2.1.6, p. 8). This is done by a succession of row reductions and/or column reductions. One of the smaller terms a_{ij} of the matrix is selected. Multiples of the i th row are subtracted from every other row so that the terms in the j th column are reduced either to zero or to non-zero remainders. Thus for the new s th row

one chooses q so that the Euclidean remainder $a_{sj} - qa_{ij}$ is either positive or negative and smaller in magnitude than a_{ij} . If the g.c.d. appears during this process either in the j th column or elsewhere in the matrix, the reduction can be stopped and the procedure of 1(a) adopted. If the column reduction continues until only one non-zero term remains, without the appearance of the g.c.d., then this one remaining term should be used in the reduction of the corresponding row. If the row reduction and possible further column reductions are completed without the appearance of the g.c.d. and there remains an isolated term (not the g.c.d.) which is the only non-zero term in its row or column, the row or column containing this term must be added to a row or column containing a term for which the isolated term is not a factor. This row or column is then reduced as before, until the g.c.d. does appear when step 1(a) is followed.

2. When the g.c.d. is located in the a_{11} position, all other terms in the first column and in the first row are reduced to zero by subtracting appropriate multiples of the first row and first column respectively.
3. After steps 1 and 2 are completed, a sub-matrix remains of order one less than that of the original matrix. The g.c.d. of this matrix must now be exhibited and moved to the leading position by the routine already established.

Note that considerable freedom is possible in the reduction of a given matrix, and the process is considerably shortened if one can choose the appropriate column or row to exhibit the required g.c.d. as rapidly as possible. Whatever routine is adopted, the canonical form will always be the same. The matrix (1p) may be different for different methods of reduction, but any two solutions so obtained will be equivalent as discussed below.

When the reduction to canonical form is completed, the equations for the x_i' read

$$\delta_1 x_1' = 0, \delta_2 x_2' = 0, \dots, \delta_r x_r' = 0 \quad \dots (8)$$

and determine the first r variables x_i' . The remaining variables may be arbitrarily chosen. The interpretation of these equations depends on the problem in hand. If one is working in a lattice which is already determined, these equations mean that a given variable x_i' must be of the form

$$x_i' = p_i \tau_i / \delta_i \quad \dots (9)$$

where τ_i is any translation of the lattice and p_i is any integer.

If it is desirable to find the simplest lattice in which a general solution of the original system can be obtained, one allots one translation to each of the equations (8) for which δ_i is not unity. These translations are linearly independent in the general case and are also linearly independent of any variables which may be left independent by the equation system.

Special cases will of course arise if linear relations are permitted between the required translations. An arbitrary number of additional independent translations may be added to those required, but the generality of the solution is not thereby increased.

The solutions x_i are then obtained from equation (7d) by the substitution of the expressions (9) and of independent parameters for the variables x_i' for which the δ -values are zero. All possible solutions are then obtained by permitting all values of $p_i < \delta_i$ and by permitting the arbitrary vectors to have components in the directions of the τ_i . This process is illustrated by the examples, and it is in this manner that one can demonstrate that the solutions obtained by different reduction routines are similar.

The three examples of Tables 2.1.9.4A–C illustrate different situations which may arise in the application of the routine described above.

TABLE 2.1.9.4A
System of Equations Valid in a Lattice

$$\begin{aligned} x_1 + 2x_2 + 3x_3 &= 0 \\ x_1 + 2x_2 - x_3 &= 0 \\ 3x_1 + 2x_2 + x_3 &= 0 \\ x_1 - 2x_2 - x_3 &= 0 \end{aligned}$$

Operation	System Matrix	Unit Matrix
g.c.d.=1	$\begin{pmatrix} 1 & 2 & 3 \\ 1 & 2 & -1 \\ 3 & 2 & 1 \\ 1 & -2 & -1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
row 1 row 1 – row 2 3(row 1) – row 3 row 1 – row 4	$\begin{pmatrix} 1 & 2 & 3 \\ 0 & 0 & 4 \\ 0 & 4 & 8 \\ 0 & 4 & 4 \end{pmatrix}$	No change
row 1 row 4 – row 2 or row 3 – 2(row 2) row 2	$\begin{pmatrix} 1 & 2 & 3 \\ 0 & 4 & 0 \\ 0 & 0 & 4 \end{pmatrix}$	No change
col. 2 – 2(col. 1) col. 3 – 3(col. 1)	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 4 \end{pmatrix}$	$\begin{pmatrix} 1 & -2 & -3 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

Solution

$$\begin{aligned} x_1' &= 0 & x_1' &= 0 & x_1 &= -p_2 \tau_2 / 2 - 3p_3 \tau_3 / 4 \\ 4x_2' &= 0 & x_2' &= p_2 \tau_2 / 4 & x_2 &= p_2 \tau_2 / 4 \\ 4x_3' &= 0 & x_3' &= p_3 \tau_3 / 4 & x_3 &= p_3 \tau_3 / 4 \end{aligned}$$

The reader who wishes to understand fully the variety of solutions presented here should write out and plot the solutions for all values of p_i in the range $0 < p_i < 4$.

TABLE 2.1.9.4B
System of Equations Valid in a Lattice

$$2x_1=0 \quad 3x_2=0 \quad 4x_3=0$$

Operations	System Matrix	Unit Matrix
g.c.d.=1	$\begin{pmatrix} 2 & 0 & 0 \\ 0 & 3 & 0 \\ 0 & 0 & 4 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
row 1+row 2	$\begin{pmatrix} 2 & 0 & 0 \\ 2 & 3 & 0 \\ 0 & 0 & 4 \end{pmatrix}$	No change
col. 2-col. 1	$\begin{pmatrix} 2 & -2 & 0 \\ 2 & 1 & 0 \\ 0 & 0 & 4 \end{pmatrix}$	$\begin{pmatrix} 1 & -1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
row 2 2(row 2)+row 1 row 3	$\begin{pmatrix} 2 & 1 & 0 \\ 6 & 0 & 0 \\ 0 & 0 & 4 \end{pmatrix}$	No change
Interchange col. 1 and col. 2	$\begin{pmatrix} 1 & 2 & 0 \\ 0 & 6 & 0 \\ 0 & 0 & 4 \end{pmatrix}$	$\begin{pmatrix} -1 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
col. 2-2(col. 1) g.c.d.=2	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 6 & 0 \\ 0 & 0 & 4 \end{pmatrix}$	$\begin{pmatrix} -1 & 3 & 0 \\ 1 & -2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
row 2+row 3	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 6 & 4 \\ 0 & 0 & 4 \end{pmatrix}$	No change
col. 2-col. 3	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 4 \\ 0 & -4 & 4 \end{pmatrix}$	$\begin{pmatrix} -1 & 3 & 0 \\ 1 & -2 & 0 \\ 0 & -1 & 1 \end{pmatrix}$
row 3+2(row 2)	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 4 \\ 0 & 0 & 12 \end{pmatrix}$	No change
col. 3-2(col. 2)	$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 12 \end{pmatrix}$	$\begin{pmatrix} -1 & 3 & -6 \\ 1 & -2 & 4 \\ 0 & -1 & 3 \end{pmatrix}$

Solution

$$\begin{aligned} x_1' &= 0 & x_1' &= 0 & x_1 &= 3p_2\tau_2/2 - p_3\tau_3/2 \\ 2x_2' &= 0 & x_2' &= p_2\tau_2/2 & x_2 &= \quad + p_3\tau_3/3 \\ 12x_3' &= 0 & x_3' &= p_3\tau_3/12 & x_3 &= -p_2\tau_2/2 + p_3\tau_3/4 \end{aligned}$$

Note that the obvious solution in terms of three translations contains and has been replaced by a less obvious and equally general solution in terms of two translations. The equally obvious solution in terms of a single translation is obtained by setting $p_2=0$.

TABLE 2.1.9.4C
System of Equations Valid in a Lattice

$$\begin{aligned} 2x_1 + x_2 + x_3 + 2x_4 &= 0 \\ x_1 + 4x_2 + 7x_3 + 9x_4 &= 0 \\ 3x_1 + 5x_2 + 5x_3 + 3x_4 &= 0 \\ 2x_1 + x_2 - 2x_3 - 6x_4 &= 0 \end{aligned}$$

Operations	System Matrix	Unit Matrix
g.c.d.=1	$\begin{pmatrix} 2 & 1 & 1 & 2 \\ 1 & 4 & 7 & 9 \\ 3 & 5 & 5 & 3 \\ 2 & 1 & -2 & -6 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$
row 1 -4(row 1)+row 2 5(row 1)-row 3 row 1-row 4	$\begin{pmatrix} 2 & 1 & 1 & 2 \\ -7 & 0 & 3 & 1 \\ 7 & 0 & 0 & 7 \\ 0 & 0 & 3 & 8 \end{pmatrix}$	No change
Rearrange columns	$\begin{pmatrix} 1 & 2 & 2 & 1 \\ 0 & 1 & -7 & 3 \\ 0 & 7 & 7 & 0 \\ 0 & 8 & 0 & 3 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{pmatrix}$
Reduce first row g.c.d.=1	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & -7 & 3 \\ 0 & 7 & 7 & 0 \\ 0 & 8 & 0 & 3 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 1 & -2 & -2 & -1 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{pmatrix}$
row 3-7(row 2) row 4-8(row 2)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & -7 & 3 \\ 0 & 0 & 56 & -21 \\ 0 & 0 & 56 & -21 \end{pmatrix}$	No change
Reduce second row and also subtract row 3 from row 4 g.c.d.=7	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 56 & -21 \\ 0 & 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & 1 & 0 \\ 1 & -2 & -16 & 5 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 7 & -3 \end{pmatrix}$
-col. 3-3(col. 4)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 7 & -21 \\ 0 & 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & -1 & 0 \\ 1 & -2 & 1 & 5 \\ 0 & 0 & -3 & 1 \\ 0 & 1 & 2 & -3 \end{pmatrix}$
col. 4+3(col. 3)	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 7 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & -1 & -3 \\ 1 & -2 & 1 & 8 \\ 0 & 0 & -3 & -8 \\ 0 & 1 & 2 & 3 \end{pmatrix}$

Solution

$$\begin{aligned} x_1' &= 0 & x_1' &= 0 & x_1 &= -p\tau/7 - 3\alpha \\ x_2' &= 0 & x_2' &= 0 & x_2 &= p\tau/7 + 8\alpha \\ 7x_3' &= 0 & x_3' &= p\tau/7 & x_3 &= -3p\tau/7 - 8\alpha \\ x_4' &= \alpha & x_4' &= \alpha & x_4 &= 2p\tau/7 + 3\alpha \end{aligned}$$

An alternative reduction of this system gives the solution

$$\begin{aligned}x_1 &= 2p'\tau/7 - 3\alpha' \\x_2 &= 8\alpha' \\x_3 &= 5p'\tau/7 - 8\alpha' \\x_4 &= -p'\tau/7 + 3\alpha'\end{aligned}$$

The fact that these two solutions are equivalent may be demonstrated by setting $\alpha' = \alpha + p\tau/7$ and $p = p'$.

Non-homogeneous systems of equations can also be analysed for solutions valid in a lattice by similar techniques. The column matrix for the constant terms must then be carried and subjected to row operations as in Tables 2.1.9.3 as well as the unit matrix.

Examples of the application of these methods to crystallography can be obtained from the theory of homometric structures.

EXAMPLE 1. The following table represents the vector distances between four atoms of equal weight in terms of their co-ordinates with respect to one of them, i.e.

0	x_1	x_2	x_3
$-x_1$	0	$x_2 - x_1$	$x_3 - x_1$
$-x_2$	$x_1 - x_2$	0	$x_3 - x_2$
$-x_3$	$x_1 - x_3$	$x_2 - x_3$	0

These distances can be rearranged to form the second distance table

0	$x_3 - x_2$	$x_2 - x_1$	$-x_3$
$x_2 - x_3$	0	x_1	$x_3 - x_1$
$x_1 - x_2$	$-x_1$	0	x_2
x_3	$x_1 - x_3$	$-x_2$	0

and therefore an arrangement homometric with the first, provided that the same difference relationship exists between the entries of the second table as existed between the corresponding entries of the first. This leads to four equations (one redundant) as follows:

$$\begin{aligned}x_1 + x_2 - 3x_3 &= 0 \\x_1 - 2x_2 - x_3 &= 0 \\2x_1 + x_2 - x_3 &= 0 \\2x_1 - 2x_2 + x_3 &= 0\end{aligned}$$

These equations have a set of solutions equivalent to

$$x_1 = -2p\tau/13, \quad x_2 = 5p\tau/13, \quad x_3 = p\tau/13$$

and lead to the same homometric pair for all integral non-zero values of p . This can easily be verified by substitution in the two distance tables above.

EXAMPLE 2. In a second case for four points the basic table can be rearranged in the form

0	$-x_2$	$x_2 - x_3$	x_3
x_2	0	$x_1 - x_2$	$-x_1$
$x_3 - x_2$	$x_2 - x_1$	0	$x_1 - x_3$
$-x_3$	x_1	$x_3 - x_1$	0

provided that

$$\begin{aligned}x_1 - 3x_2 + x_3 &= 0 \\x_1 + x_2 + x_3 &= 0 \\3x_1 - x_2 - x_3 &= 0 \\x_1 + x_2 - 3x_3 &= 0\end{aligned}$$

These equations have a set of solutions equivalent to

$$x_1 = -p_1\tau_1/4 - p_2\tau_2/4, \quad x_2 = p_1\tau_1/4, \quad x_3 = p_2\tau_2/4$$

and to the same homometric pair of structures for p_1p_2 both odd. All other cases lead to identical pairs.

2.1.10. Transcendental Equations

2.1.10.1. SINGLE VARIABLE

The general method for the solution of the equation

$$f(x) = 0 \quad \dots (1)$$

depends on the location of an approximation x_0 to a root and on the improvement of that approximation by means of the first two terms of the Taylor expansion

$$f(x_0 + \Delta x) \approx f(x_0) + f'(x_0)\Delta x \quad \dots (2)$$

Thus, if x_0 is an approximate value of a solution to (1), then $x_1 = x_0 + \Delta x$ is an improved value of this solution if Δx is calculated from

$$\Delta x = -f(x_0)/f'(x_0) \quad \dots (3)$$

This method of improving a root is known as the *Newton-Raphson method*. It is most effective when $|f'(x_0)|$ is large. It should be avoided if $f'(x_0)$ is difficult to calculate.

The expression (3) can be modified by setting ($x_1 > x_0$)

$$f'(x_0) \approx \frac{f(x_1) - f(x_0)}{x_1 - x_0}$$

to obtain

$$\Delta x = -f(x_0)(x_1 - x_0)/[f(x_1) - f(x_0)] \quad \dots (4)$$

This will give rise to an improved root provided x_1 and x_0 are close to each other and to the root. It is most effective when $f(x_1)$ and $f(x_0)$ are of opposite sign. The result of equation (4) is known as *the rule of false position* or *regula falsi*.

A third approach, called the *method of iteration*, results from rewriting (1) in the form†

$$x = \phi(x) \quad \dots (5)$$

Then, if x_p is an approximate root of (5), x_{p+1} given by

$$x_{p+1} = \phi(x_p) \quad \dots (6)$$

will be a better approximation than x_p provided that $|\phi'(x)| < 1$ in the neighbourhood of the desired root. There are usually several ways in which (5) can be written from (1).

For variations on the methods which we have included and for a detailed discussion of their accuracy, reference must be made to [24], [25] and [26].

It is difficult to lay down a routine for the solution

† The more general form $\phi_1(x) = \phi_2(x)$ can also be used as the basis of an iterative procedure, but the one given in the text is the more usual.

2.1. ALGEBRA

of a transcendental equation or for the selection of the method to be used. If the function and its derivative are both easily computed, the Newton-Raphson method is probably the most profitable in general,

provided $f'(x)$ is not too small. Otherwise an iterative process is probably the best attack, but then the selection of the form for (5) is a matter for trial and error and/or for the experience of the computer.

TABLE 2.1.10.1A

Example of the Newton-Raphson Method

Compute the solution of the equation

$$\frac{\sin x}{x} = \frac{1}{2} \quad \dots (7)$$

i.e. the half-value breadth of the one-dimensional interference function.

Consider $f = 2 \sin x - x = 0$

$$\frac{df}{dx} = 2 \cos x - 1$$

Using (3), when x_0 is a possible solution, $x_0 + \Delta x$ is a better solution if

$$\Delta x = -\frac{(2 \sin x_0 - x_0)}{(2 \cos x_0 - 1)} \quad \dots (8)$$

In solving this equation eight-place trigonometric tables with argument in radians were used. As initial value we assume $x = 1.732$, obtained from the solution of the approximate equation

$$(x - x^3/3!)/x - \frac{1}{2} = 0, \text{ i.e. } x^2 = 3 \quad \dots (9)$$

The approximation routine is then as follows:

x	$\sin x$	$\cos x$	$2 \sin x - x$	$2 \cos x - 1$	Δx
1.732	0.9870	-0.1605	+0.2420	-1.3210	+0.1832
1.9152	0.9412	-0.3376	-0.0328	-1.6752	-0.0196
1.8956	0.94771328	-0.31912269	-0.00017344	-1.63824538	-0.00010586
1.89549414	0.94774705	-0.31902237	-0.00000004	-1.63804474	-0.00000002
1.89549412	0.94774706		0.00000000		

The solution $x = 1.895494$ is clearly accurate to six decimal places. The two additional places may be in error, since linear interpolation was used on a three-place argument. Correctly, the last two digits in the above table should be 26 instead of 12.

TABLE 2.1.10.1B

Example of the Rule of False Position

Consider the equation

$$\frac{3}{x^3} (\sin x - x \cos x) = \frac{1}{2} \quad \dots (10)$$

involved in finding the half-value breadth for the diffraction function for a sphere.

An approximate solution can be obtained by expansion in series, i.e.

$$\begin{aligned} 1 &\approx \frac{6}{x^3} \left[\left(x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} \right) - x \left(1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} \right) \right] \\ &= \frac{6}{x^3} \left[\frac{x^3}{2!} \left(1 - \frac{1}{3} \right) - \frac{x^5}{4!} \left(1 - \frac{1}{5} \right) + \frac{x^7}{6!} \left(1 - \frac{1}{7} \right) \right] \\ &= 2 - \frac{x^2}{5} + \frac{x^4}{140} \end{aligned}$$

We therefore solve

$$x^4 - 28x^2 + 140 = 0$$

to find the approximate solution

$$x = 2.55$$

Since the solution is remote from $x = 0$, we write (10) in the form

$$f(x) = \sin x - x \cos x - x^3/6 = 0 \quad \dots (11)$$

This equation could be solved by the Newton-Raphson method, but it is perhaps simpler to use the rule of false position. The successive approximations can then be tabulated as follows:

	x	$\cos x$	$\sin x$	$x^3/6$	$f(x)$	Δx
x_0	2.5	-0.8011	0.5985	2.6042	-0.0030	
x_1	2.49	-0.7951	0.6065	2.5730	+0.0133	-0.0018
x_0	2.4982	-0.800065	0.599913	2.598546	+0.00008938	
x_1	2.4983	-0.800125	0.599833	2.598858	-0.00007271	+0.000055
x_0	2.498255	-0.80009806	0.59986923	2.59871734	+0.00000086	
x_1	2.498256	-0.80009866	0.59986843	2.59872046	-0.00000075	+0.00000053

Final value $x = 2.4982555$

TABLE 2.1.10.1C

Examples of the Method of Iteration

1. *Square Roots.* Consider $x^2=a$. This equation suggests iteration in the form

$$x_1 = \frac{a}{x_0}$$

but this relation is clearly non-convergent, since $|\phi'(x)|=1$ at the solution. If, however, we follow Newton and write

$$x_1 = \frac{1}{2} \left(x_0 + \frac{a}{x_0} \right) \quad \dots (12)$$

the iteration process will converge. Note that the number of correct digits doubles (approximately) at each step.

Calculation of $\sqrt{\pi}$ (nine decimal places)

By slide rule $\sqrt{\pi}=1.772=x_0$. Using (12) by machine we get

$$x_1 = 1.772453909$$

$$x_2 = 1.772453851 \text{ (correct to 9 places)}$$

2. *Higher Integral Roots.* The solution of $x^n=a$ is similarly obtained by iteration of the expression

$$x_1 = \frac{1}{n} \left[(n-1)x_0 + \frac{a}{x_0^{n-1}} \right] \quad \dots (13)$$

3. In determining the extrema of $y=\sin x/x$ we find

$$\frac{dy}{dx} = \frac{x \cos x - \sin x}{x^2}$$

and we desire solutions of the equation

$$x = \tan x \quad \dots (14)$$

which suggest an iteration procedure. However, $\frac{d}{dx}(\tan x) = \sec^2 x$, which is always greater than unity, so that the iteration will not converge. If we rewrite the equation in the form

$$x = \tan^{-1} x \quad \dots (15)$$

we note that $\frac{d}{dx}(\tan^{-1} x) = 1/(1+x^2)$ and we can expect convergence for large x . The non-zero solutions of (14) are clearly near $(2k+1)\pi/2$. For the solution near $3\pi/2$ the iteration procedure is as follows (using tables with argument in degrees and minutes):

x	$\tan^{-1} x$		$180^\circ + \tan^{-1} x$
4.7124	78° 1.3'	78.02°	258.02°
4.5033	77° 28.8'	77.48°	257.48°
4.4939	77° 27.29'	77.4548°	257.4548°
4.493433	77° 27.2075'	77.4535°	257.4535°
4.493411	77° 27.2039'	77.4534°	257.4534°
4.493409	77° 27.2036'	77.4534°	

2.1.10.2. SIMULTANEOUS EQUATIONS IN SEVERAL VARIABLES

Suppose that $f_1(x,y)=0$ and $f_2(x,y)=0$ are to be satisfied simultaneously, and that we have an approximate solution x_0, y_0 . Then clearly an improved solution $x_0+\Delta x, y_0+\Delta y$ is obtained if the equations

$$\left. \begin{aligned} f_1(x_0, y_0) + \frac{\partial f_1}{\partial x} \Delta x + \frac{\partial f_1}{\partial y} \Delta y &= 0 \\ f_2(x_0, y_0) + \frac{\partial f_2}{\partial x} \Delta x + \frac{\partial f_2}{\partial y} \Delta y &= 0 \end{aligned} \right\} \quad \dots (1)$$

are satisfied, the derivatives being calculated numerically for the approximate solution x_0, y_0 . This is the counterpart of the Newton-Raphson method for two variables. It can be extended to any number of variables in an obvious manner.

In two variables the rule of false position takes the form

$$\left. \begin{aligned} f_1(x_0, y_0) + [f_1(x_1, y_0) - f_1(x_0, y_0)] \frac{\Delta x}{(x_1 - x_0)} \\ + [f_1(x_0, y_1) - f_1(x_0, y_0)] \frac{\Delta y}{(y_1 - y_0)} &= 0 \\ f_2(x_0, y_0) + [f_2(x_1, y_0) - f_2(x_0, y_0)] \frac{\Delta x}{(x_1 - x_0)} \\ + [f_2(x_0, y_1) - f_2(x_0, y_0)] \frac{\Delta y}{(y_1 - y_0)} &= 0 \end{aligned} \right\} \quad \dots (2)$$

and can be extended to any number of variables.

TABLE 2.1.10.2

Solution of Simultaneous Transcendental Equations

Consider the two-parameter, one-dimensional diffraction problem in which the third and the fifth orders are both missing experimentally. The structure factors are written

$$F(3) = 2\{0.39 \cos 2\pi 3x_1 + 0.60 \cos 2\pi 3x_2\} = 0 \quad \dots (3a)$$

$$F(5) = 2\{0.24 \cos 2\pi 5x_1 + 0.40 \cos 2\pi 5x_2\} = 0 \quad \dots (3b)$$

From equation (1) we may write

$$6\pi(0.39) \sin 2\pi 3x_1 \Delta x_1 + 6\pi(0.60) \sin 2\pi 3x_2 \Delta x_2 = \frac{1}{2}F(3) \quad \dots (4a)$$

$$10\pi(0.24) \sin 2\pi 5x_1 \Delta x_1 + 10\pi(0.40) \sin 2\pi 5x_2 \Delta x_2 = \frac{1}{2}F(5) \quad \dots (4b)$$

It is clear that equation (3a) has solutions at $x_1=(2k_1+1)/12$; $x_2=(2k_2+1)/12$; and along sinuous curves through these points in the general direction of the x_1 axis. Equation (3b) has solutions at $x_1=(2l_1+1)/20$; $x_2=(2l_2+1)/20$; and along curves joining these points, again in the general direction of the x_1 axis. We can sketch plots of these curves by noting that for $x_1=2k_1/12=k_1/6$, equation (3a) has solutions where $\cos 2\pi 3x_2 = -(-1)^{k_1} 0.39/0.60$. Also that equation (3b) has solutions for $x_1=l_1/10$ where

TABLE 2.1.10.2 (continued)
Solution of Simultaneous Transcendental Equations

Arguments in Cycles						Determinant of Equations (4)	$\frac{1}{2}F(3)$ $\frac{1}{2}F(5)$	$\cos 2\pi 3x_1$ $\cos 2\pi 3x_2$ $\cos 2\pi 5x_1$ $\cos 2\pi 5x_2$		D	$D\Delta x_1$ $D\Delta x_2$		Δx_1 Δx_2
x_1	x_2	$3x_1$	$3x_2$	$5x_1$	$5x_2$								
0.050	0.250	0.150	0.750	0.250	0.250	5.947	0.2293	0.588	0	160.01	2.8814	0.0180	
						7.540	0	0	0		-1.7289	-0.0108	
0.0680	0.2392	0.2040	0.7176	0.3400	0.1960	7.042	-0.0100	0.285	-0.202	153.99	-0.0675	-0.0004	
						6.364	0.0046	-0.536	0.333		0.0960	0.0006	
0.0676	0.2398	0.2028	0.7194	0.3380	0.1990		-0.0007	0.292	-0.191				
							0.0000	-0.525	0.315				

$\cos 2\pi 5x_2 = -(-1)^{1/4} 0.24/0.40$. Rough sketches indicate that in addition to the obvious solution at $x_1 = x_2 = \frac{1}{4}$ there are three other solutions in the range $0 < x_1, x_2 < \frac{1}{4}$. The first of these near $x_1 = 0.050$, $x_2 = 0.250$, is refined as shown in the table on page 25.

In this calculation an extra place is carried in the x_1, x_2 values to give greater accuracy after multiplication by the order numbers. The sine and cosine values are read from three-figure tables such as those in Section 8.3. The coefficients of the determinant of equations (4) are then entered in the appropriate column, and the solutions of equations (4) are calculated by the methods of 2.1.9.3 (page 17). In this case it is clear that a solution $x_1 = 0.068$, $x_2 = 0.240$ is correct to three places in decimal fractions of the cell dimensions. The reader who wishes may find two other roots by taking as initial values $x_1 = 0.150$, $x_2 = 0.050$, and also $x_1 = 0.250$ and $x_2 = 0.050$. All roots are, of course, repeated according to the symmetry of expressions (3).

2.1.11. Polynomial Equations

All the methods which have been devised for the solution of transcendental equations can also be applied to the solution of polynomial equations, but the latter have a number of special properties, and in consequence special methods which can be applied to their solution.

2.1.11.1. GENERAL RESULTS

The equation

$$f(x) = a_0x^n + a_1x^{n-1} + \dots + a_{n-1}x + a_n = 0 \quad \dots (1)$$

has n roots. If the coefficients a_i are all real, the roots are either real or occur in conjugate complex pairs. If the coefficients a_i are rational or rationally dependent, the roots are either rational or occur in conjugate irrational pairs ($A \pm \sqrt{B}$, A and B rational).

If the coefficients are complex, the roots will in general be complex. Some of the results given below will be valid for complex coefficients if careful attention is paid to the proper interpretation of the algebraic operations for complex numbers; otherwise it may be best to expand the equation into simultaneous equations with real coefficients for the real and imaginary parts of the unknown.

2.1.11.2. LOCATION OF ROOTS

The following theorems serve to locate the roots of the equation (1).

(a) *Descartes' Rule of Signs*. No equation can have more positive roots than there are changes in sign from $+$ to $-$ and from $-$ to $+$ in the sequence of coefficients a_0, a_1, \dots, a_n of $f(x)$.

No equation can have more negative roots than there are changes in sign in the sequence of coefficients of the function $f(-x)$.

(b) If two numbers a and b , substituted for x in the polynomial $f(x)$, give results with contrary signs, an odd number of real roots lies between them; and if they give results with the same sign, either no real root or an even number of real roots lies between them.

(c) The theorems of Fourier and Budan locate the roots in terms of the changes of sign of $f(x)$ and of its derivatives. For details, reference is made for example to [21].

(d) A set of functions called *Sturm's functions* can be calculated which permit the exact location of all real roots of a polynomial and the determination of their multiplicity. Discussion of these functions is given in [18], [21], [24] and [26]; a useful routine for their calculation is given in [18].

2.1.11.3. SPECIAL EQUATIONS

The *quadratic equation*

$$ax^2 + 2bx + c = 0 \quad \dots (2)$$

has the two solutions

$$x = [-b \pm \sqrt{(b^2 - ac)}]/a \quad \dots (3)$$

If the coefficients are all real, there are two unequal real solutions when $b^2 - ac > 0$; two equal real solutions when $b^2 - ac = 0$; and two conjugate complex solutions when $b^2 - ac < 0$.

The *cubic equation*

$$ax^3 + 3bx^2 + 3cx + d = 0 \quad \dots (4)$$

is reduced to standard form by dividing the coefficients

$$\text{by } a \text{ and by setting } x = y - b/a \quad \dots (5)$$

$$\text{when we obtain } y^3 + 3Hy + G = 0 \quad \dots (6a)$$

$$\text{in which } H = (ac - b^2)/a^2 \quad \dots (6b)$$

$$\text{and } G = (a^2d - 3abc + 2b^3)/a^3 \quad \dots (6c)$$

We assume a, b, c, d all real and use the notation $H = s_h h$ and $G = s_g g$, where $h = |H|$ and $g = |G|$. The three cases of interest are summarized in Table 2.1.11.3. These solutions require the use of tables of trigonometric functions and of hyperbolic functions and are limited in accuracy by that of the available tables. Solutions obtained by these methods can be refined by the methods of 2.1.10.1 (p. 22) or by Horner's method (2.1.11.4, p. 28).

Any equation of the form (1) in which

$$a_m = a_{n-m} \quad \dots (7a)$$

is called a *reciprocal equation of the first class*, and one in which

$$a_m = -a_{n-m} \quad \dots (7b)$$

is called a *reciprocal equation of the second class*. If α is a root of a reciprocal equation, $1/\alpha$ is also a root.

Any reciprocal equation of the first class of odd degree has one root $x = -1$, and consequently a factor $(x+1)$ can be removed from the equation. Any reciprocal equation of the second class and odd degree has $x = 1$ as a root, and a factor $(x-1)$ can be removed.

Any reciprocal equation of the second class and even degree has the two roots $x=\pm 1$ and the factor (x^2-1) . The result in each of these three cases is a reciprocal equation of the first class of even degree, which is thus the standard form for reciprocal equations, i.e.

$$a_0x^{2m}+a_1x^{2m-1}+\dots+a_mx^m+\dots+a_1x+a_0=0 \quad \dots(8a)$$

This may be written in the form

$$a_0V_m+a_1V_{m-1}+\dots+a_{m-1}V_1+a_m=0 \quad \dots(8b)$$

$$\text{in which } V_p=x^p+1/x^p \quad (p \geq 0) \quad \dots(8c)$$

$$\text{and } V_{p+1}=V_pZ-V_{p-1} \quad \dots(8d)$$

$$\text{where } Z=x+1/x \quad \dots(8e)$$

The algebraic form for each V_p is as follows:

$$\begin{aligned} V_1 &= Z \\ V_2 &= Z^2 - 2 \\ V_3 &= Z^3 - 3Z \\ V_4 &= Z^4 - 4Z^2 + 2 \\ V_5 &= Z^5 - 5Z^3 + 5Z \\ V_6 &= Z^6 - 6Z^4 + 9Z^2 - 2 \end{aligned} \quad \dots(8f)$$

in which the algorithm tells us that the numerical value of the coefficient of a given term is obtained from the sum of that immediately above and that two above and one to the left (a Knight's move, neglecting signs). The signs alternate in a given equation and propagate vertically. The use of the substitutions (8f) leads to an equation of degree m in Z . From the m roots Z_i of this equation, one obtains the $2m$ roots of the standard equation (8a) by the solution of the quadratic

$$x^2 - Z_ix + 1 = 0 \quad \dots(8g; \text{ cf. } 8e)$$

that is to say

$$x = \frac{1}{2}[Z_i \pm \sqrt{(Z_i^2 - 4)}] \quad \dots(8h)$$

When Z_i is real, (8h) applied directly will give two values for x which will of course be reciprocals of each other. When Z_i is complex, the expression under the root will also be complex, and must be so treated in extracting the root. Thus (8h) will apparently lead to four roots for (8g), which is, of course, illusory. They will consist of two equal pairs, and only two different roots will be obtained.

TABLE 2.1.11.3
Solution of the Cubic $y^3+3Hy+G=0$
Notation: $h=|H|$; $g=|G|$; $H=s_hh$; $G=s_gg$

Equation	Conditions	Roots
I. $y^3+3hy+s_gg=0$	$\sinh 3\theta=g/2h^{3/2}$	$-2s_g\sqrt{h} \sinh \theta$; $s_g\sqrt{h}(\sinh \theta \pm i\sqrt{3} \cosh \theta)$
II. $y^3-3hy+s_gg=0$	$g^2>4h^3$; $\cosh 3\theta=g/2h^{3/2}$	$-2s_g\sqrt{h} \cosh \theta$; $s_g\sqrt{h}(\cosh \theta \pm i\sqrt{3} \sinh \theta)$
III. $y^3-3hy+s_gg=0$	$g^2<4h^3$; $\cos 3\theta=g/2h^{3/2}$	$-2s_g\sqrt{h} \cos \theta$; $s_g\sqrt{h}(\cos \theta \pm \sqrt{3} \sin \theta)$
		$\sqrt{3}=1.7320508$

Special Cases

$G^2+4H^3>0$. One real, two conjugate complex roots (I or II).

$G^2+4H^3=0$; $G^2=-4H^3$. Three real roots, two equal $[-2s_g\sqrt{h}, s_g\sqrt{h}, s_g\sqrt{h}]$.

$G^2=4H^3=0$. Three equal real roots [$y=0$].

$G^2+4H^3<0$. Three unequal real roots (III).

EXAMPLE. Consider the cubic

$$6x^3-45x^2+108x-82=0$$

Here $-b/a=5/2$, and Horner's scheme (2.1.11.4, p. 28, $r=5/2$, $h=y$) for the reduction to standard form is written

$$\begin{array}{rrrr} 6 & -45 & +108 & -82 \\ & -30 & 33 & +1/2 \\ & -15 & -9/2 & \\ & 0 & & \end{array} \quad (5/2)$$

so that the reduced cubic is

$$y^3-(3/4)y+(1/12)=0$$

with $g=1/12$; $h=1/4$; $s_g=+1$; and $g^2/4h^3=1/9$ (Type

III). We then have $\cos 3\theta=1/3$, i.e. $3\theta=70.52^\circ$ (using 5-place tables) and $\theta=23.51^\circ$. We then have

$$\begin{array}{lll} \cos \theta=0.91699 & \sqrt{3} \sin \theta=0.69092 & x=y+5/2 \\ \sin \theta=0.39890 & \sqrt{h}=1/2 & \\ y_1=-0.91699 & x_1=1.58301 & \\ y_2=0.11304 & x_2=2.61304 & \\ y_3=0.80396 & x_3=3.30396 & \end{array}$$

The accuracy to be obtained by this method depends on the accuracy of the tables which are used. Reference to the more exact solution of this equation (Table 2.1.11.4B) indicates that the above solution is exact as far as it is given.

After the solution of the standard equation (6a) has been completed, the solution of the original equation (5a) is of course obtained by substitution of the y solutions in (5b).

2.1.11.4. HORNER'S REDUCTION FOR A POLYNOMIAL EQUATION

If we know an approximate root r for equation (1) we can improve this approximation by calculating the function $f(r+h)$ as a polynomial in h giving an equation in h which can be solved for its smallest root. The process for calculating the coefficients of powers of h in $f(r+h)$ from the corresponding coefficients of powers of x in $f(x)$ has been schematized by Horner (see [23], [25]). Horner's scheme for the quintic

$$f(x) = a_0x^5 + a_1x^4 + a_2x^3 + a_3x^2 + a_4x + a_5 = 0$$

is exhibited in Table 2.1.11.4A. It can readily be written down for any other degree by following a similar scheme.

The use of Horner's reduction in locating more precisely an approximately known root is illustrated in Table 2.1.11.4B. When the Horner reduction is completed to the accuracy desired, the remaining portion of the equation can be solved for other roots of the equation. Comment is made on some practical points in the course of the example of Table 2.1.11.4B.

TABLE 2.1.11.4A
Horner's Reduction

$f(x) = a_0x^5 + a_1x^4 + a_2x^3 + a_3x^2 + a_4x + a_5$					
a_0	a_1	a_2	a_3	a_4	a_5
	$\frac{ra_0}{b_1 = ra_0 + a_1}$	$\frac{rb_1}{b_2 = rb_1 + a_2}$	$\frac{rb_2}{b_3}$	$\frac{rb_3}{b_4}$	$\frac{rb_4}{b_5}$
	$\frac{ra_0}{c_1 = ra_0 + b_1}$	$\frac{rc_1}{c_2 = rc_1 + b_2}$	$\frac{rc_2}{c_3}$	$\frac{rc_3}{c_4}$	
	$\frac{ra_0}{d_1}$	$\frac{rd_1}{d_2}$	$\frac{rd_2}{d_3}$		
	$\frac{ra_0}{e_1}$	$\frac{re_1}{e_2}$			
	$\frac{ra_0}{f_1}$				
$f(r+h) = a_0h^5 + f_1h^4 + e_2h^3 + d_3h^2 + c_4h + b_5$					

NOTE. In desk machine calculation by Horner's method the only entries which need be written are

a_0	a_1	a_2	a_3	a_4	a_5	(r)
	b_1	b_2	b_3	b_4	b_5	
	c_1	c_2	c_3	c_4		
	d_1	d_2	d_3			
	e_1	e_2				
	f_1					

All other entries in the above table can be handled in the machine.

TABLE 2.1.11.4B

Use of Horner's Method in the Solution of a Polynomial Equation

Consider the cubic

$$f(x) = 6x^3 - 45x^2 + 108x - 82 = 0 \quad \dots (1)$$

and the derivative of $f(x)$, i.e.

$$f'(x) = 18x^2 - 90x + 108 \quad \dots (2)$$

At $x=0$, $f(x)=-82$ and $f'(x)=108$. At $x=1$ these functions are -13 and $+36$ respectively. Thus there is clearly a root near to (and greater than) 1. We use Horner's reduction to make the substitution $x=1+h_1$ as follows:

6	-45	108	-82	(1)
	6	-39	69	
	-39	69	-13	
	6	-33		
	-33	36		
	6			
	-27			

and the equation for h_1 is

$$6h_1^3 - 27h_1^2 + 36h_1 - 13 = 0 \quad \dots (3a)$$

which may be rewritten

$$36h_1 = 13 + 27h_1^2 - 6h_1^3 \quad \dots (3b)$$

A first approximation is $h_1 = 13/36 = 0.36$, and this will clearly be low. It is possible at this stage to make successive approximations to solve (3b), but experience indicates that it is perhaps more profitable to guess and to continue the Horner reduction of equation (3a), since the convergence of (3b) may be very slow at early stages. We shall make this guess as $h_1 = 0.4 + h_2$.

NOTE. We must here make some sort of decision as to the accuracy to which calculations will be carried out. We have here quite arbitrarily decided that this equation shall be satisfied to six decimal places. The question of accuracy of solution is discussed in [22] and [24]; but these discussions are very complicated, and in general much must be left to the instinct of the computer in relation to the problems which he has under consideration. When once such a decision is made, approximations short of this accuracy should not be made, since they may lead to difficulties.

The reduction of the roots by 0.4 is then

6	-27	36	-13	(0.4
	2.4	-9.84	10.464	
	-24.6	26.16	-2.536	
	2.4	-8.88		
	-22.2	17.28		
	2.4			
	-19.8			

and the equation for h_2 is

$$6h_2^3 - 19.8h_2^2 + 17.28h_2 - 2.536 = 0 \quad \dots (4)$$

The approximate solution of this equation, i.e. $h_2=2.536/17.28=0.146$, indicates that we have underestimated h_1 . We also note that h_2 is probably low, since the term in h_2^2 has the same sign as the constant. We therefore choose $h_2=0.15+h_3$. Note that we now omit the intermediate step in each Horner reduction, as can always be done on a calculating machine, and write simply

$$\begin{array}{r} 6 \quad -19.8 \quad 17.28 \quad -2.536 \quad (0.15 \\ \quad -18.9 \quad 14.445 \quad -0.36925 \\ \quad -18.0 \quad 11.745 \\ \quad -17.1 \end{array}$$

We thus obtain

$$6h_3^3 - 17.1h_3^2 + 11.745h_3 - 0.36925 = 0 \quad \dots (5a)$$

From this we obtain as first approximation $h_3 \approx 0.0314$. At this stage it is profitable to consider the equation

$$11.745h_3 = 0.36925 + 17.1h_3^2 \quad \dots (5b)$$

If we insert the first approximation into the right-hand side of (5b) and recalculate h_3 , we find $h_3 \approx 0.0329$; this is clearly high, from the sign of the h_3^3 term. We assume $h_3 = 0.032 + h_4$ and the next Horner approximation takes the form

$$\begin{array}{r} 6 \quad -17.1 \quad 11.745 \quad -0.36925 \quad (0.032 \\ \quad -16.908 \quad 11.203944 \quad -0.010724 \\ \quad -16.716 \quad 10.669032 \\ \quad -16.524 \end{array}$$

and the equation for h_4 becomes

$$6h_4^3 - 16.524h_4^2 + 10.669032h_4 - 0.010724 = 0 \quad \dots (6)$$

It is now very clearly possible to obtain a solution to (6) which is accurate to the limits we have set. The first approximation leads to $h_4 = 0.001005$, and if we take into account the term in h_4^2 we obtain the slightly better value with 6 in the last digit. We thus obtain the root as

$$x = 1 + h_1 + h_2 + h_3 + h_4 = 1 + 0.4 + 0.15 + 0.032 + 0.001006 = 1.583006$$

We now verify the whole calculation by the Horner reduction:

$$\begin{array}{r} 6 \quad -45 \quad 108 \quad -82 \quad (1.583006 \\ \quad -35.501964 \quad 51.800178 \quad -0.000007 \\ \quad -26.003928 \quad 10.635804 \\ \quad -16.505892 \end{array}$$

which indicates that the correct root is probably closer to 1.583007.

The equation which remains, i.e.

$$6h_5^3 - 16.505892h_5^2 + 10.635804h_5 = 0 \quad \dots (7)$$

can, after h_5 is divided out, be used to find the other roots of the equation under consideration. In this case we have to solve a quadratic; in other cases we may have to start again on a Horner reduction for the smallest root.

2.1.11.5. GRAEFFE'S ROOT-SQUARING METHOD

This method, which depends on forming the equation whose roots are successively higher binary powers of the roots of the original equation, serves to locate all the roots of a given equation. It is not possible to give a full account of this method in the space available in these tables. Reference is therefore made to [24], [25] and [26].

For theoretical background of Section 2.1.11 generally see [21]. For numerical methods see [18], [22]–[26].

2.1.12. Groups

2.1.12.1. GROUP POSTULATES

A *group* consists of a set of mathematical objects, called the *elements* of the group, which satisfy the following four *group postulates*:

- I. Between the elements of the group there is uniquely defined a method of connection called *multiplication*. Under multiplication, any two elements A (called the *pre-factor*) and B (called the *post-factor*) define a third element of the group C , called the *product*, i.e. $AB = C$.
- II. The associative law must hold for multiplication, i.e. $A(BC) = (AB)C$.
- III. There exists one and only one element, called the *identity element*, E , such that for any other element A of the group $AE = EA = A$.
- IV. Every element of the group has a unique reciprocal, i.e. for a given element A there exists one and only one element $B = A^{-1}$ such that $AB = BA = E$.

It is important to note that:

1. Group multiplication has no necessary connection with arithmetical or algebraic multiplication.
2. The commutative law need not hold in group multiplication, i.e. the product AB (i.e. the operation B followed by the operation A) is not necessarily equal to BA (i.e. the operation A followed by the operation B).
3. It follows from I that the product of an element with itself (i.e. $AA = A^2$) must also be an element of the group.

2.1.12.2. DEFINITIONS

1. An *abstract group* is concerned only with the relationships of a set of operations as apart from their nature.
2. A group for which the commutative law (i.e. $AB = BA$) holds for all elements is said to be *Abelian*.
3. A group which contains n elements is said to be of *order* n . The order of a group may be finite or infinite.

4. If among the n elements of a group it is possible to find a subset of m elements which themselves satisfy the group postulates, these elements form a *sub-group* of the original group. Every sub-group must contain the identity element. The order m of a sub-group must be a factor of the order n of the group which contains it.
5. If r is the smallest integer for which $X^r=E$, r is called the *order of the element* X , and the r elements $X, X^2, \dots, X^{r-1}, X^r=E$ form the *period* of X . The period of any element of a finite group is either the group itself, in which case the group is called a *cyclic group*, or the period is a (cyclic) sub-group of the group containing the element.
6. Two groups G and G' are said to be *simply isomorphous*[†] if to each element A, B, C, \dots of G there corresponds one and only one element A', B', C', \dots of G' so that if $AB=C$ then $A'B'=C'$ for every product. If several elements of one group correspond to a single element of the second, then the groups are said to be *multiply isomorphous*.
7. If to every element of an abstract group there corresponds a member of a set of concrete mathematical objects (such as numbers, matrices or geometrical operations) in such a way that the concrete objects form a group isomorphous with the abstract group, then the concrete group is said to form a *representation*[‡] of the abstract group.
8. The properties of the elements of a group are most conveniently represented by a *group multiplication table*. In such a table the elements of the group are listed in the top row (led by the identity) and in this position are considered as post-factors. In the first column (with the identity in common with the first row) the elements are represented and considered as pre-factors. An entry of the table is then the product of the corresponding entry in the first column (pre-factor) with the corresponding entry of the first row (post-factor). The order of the elements (other than identity) in the first column is not necessarily dependent on that in the first row. It is, however, usual to write the inverse of an element in the first column in the position corresponding to the element in the first row. In this way the identity always appears along the diagonal of the table and the table is always anti-symmetric about the diagonal.

2.1.12.3. RESULTS AND EXAMPLES OF GROUP THEORY

1. For every order n there is always a cyclic group.
2. For every prime number p there is one and only one group of order p and that is the cyclic group of order p , and the only sub-group of such a group is the identity operation E .
3. The cyclic groups are Abelian.

4. There is, of course, only one crystallographic group of order unity, i.e. 1.
5. The three crystallographic groups of order two, i.e. $\bar{1}, 2, m$, are simply isomorphous with the cyclic abstract group of order two.
6. The group table for the cyclic groups is typified by that of order four, which is as follows:

E	A	A^2	A^{-1}	
A^{-1}	E	A	A^2	
A^2	A^{-1}	E	A(1)
A	A^2	A^{-1}	E	

Groups isomorphous with this abstract group include:

- (i) The group associated with the symbol i under algebraic multiplication which has the table

1	i	-1	$-i$	
$-i$	1	i	-1	
-1	$-i$	1	i(2)
i	-1	$-i$	1	

The identity operation is, of course, the number 1. The group (2) is simply isomorphous with the group (1).

- (ii) The group of all integers (positive and negative and zero) under addition modulo 4 (2.1.5, p. 7) as group multiplication operation. The identity operation is 0, and the group multiplication table reads:

0	1	2	-1	
-1	0	1	2	
2	-1	0	1(3)
1	2	-1	0	

This is clearly an infinite group which is multiply isomorphous with the group (1).

- (iii) The crystallographic three-dimensional point groups (Vol. I, 3.6) which are simply isomorphous with (1) are 4 and $\bar{4}$, which have group tables

1	4	2	4^{-1}	
4^{-1}	1	4	2	
2	4^{-1}	1	4(4)
4	2	4^{-1}	1	

and

1	$\bar{4}$	2	$\bar{4}^{-1}$	
$\bar{4}^{-1}$	1	$\bar{4}$	2	
2	$\bar{4}^{-1}$	1	$\bar{4}$(5)
$\bar{4}$	2	$\bar{4}^{-1}$	1	

in which the operations are represented by powers of their Hermann-Mauguin symbols.

[†] The use of the term isomorphous in group theory should not be confused with the use of the same term in crystallography.

[‡] For discussion of the theory of representations see [28] and [30].

7. There is a second abstract group of order four, represented by the table

1	A	B	C	
A	1	C	B	
B	C	1	A(6)
C	B	A	1	

This abstract group has three crystallographic representations: $2/m$, 222 , and $mm2$, for which the tables are respectively:

$2/m$			
1	m	2	$\bar{1}$
m	1	$\bar{1}$	2
2	$\bar{1}$	1	m
$\bar{1}$	2	m	1
222			
1	$2 \cdot \cdot$	$\cdot 2 \cdot$	$\cdot \cdot 2$
$2 \cdot \cdot$	1	$\cdot \cdot 2$	$\cdot 2 \cdot$
$\cdot 2 \cdot$	$\cdot \cdot 2$	1	$2 \cdot \cdot$
$\cdot \cdot 2$	$\cdot 2 \cdot$	$2 \cdot \cdot$	1
$mm2$			
1	$m \cdot \cdot$	$\cdot m \cdot$	$\cdot \cdot 2$
$m \cdot \cdot$	1	$\cdot \cdot 2$	$\cdot m \cdot$
$\cdot m \cdot$	$\cdot \cdot 2$	1	$m \cdot \cdot$
$\cdot \cdot 2$	$\cdot m \cdot$	$m \cdot \cdot$	1

In this group and in its representations there are three sub-groups of order two which are independent, as is indicated by the dots, which locate the Hermann-Mauguin symbols with respect to the axes with which they may have been arbitrarily associated. Such distinctions have been omitted for the sake of simplicity in the tables of Vol. I (Table 3.6.2), in which only one sub-group 2 has been indicated instead of the three which do occur.

8. The only crystallographic group of order three is the cyclic group 3.
9. The three crystallographic point groups $\bar{3}$, 6 and $\bar{6}$ are simply isomorphous with the cyclic group of order six and as such contain one sub-group of order two ($\bar{1}$, 2 and m respectively) and one sub-group of order three (in all cases the point group 3).
10. The two non-cyclic crystallographic point groups of order six, 32 and $3m$, are simply isomorphous and have the common group table:

1	3	3^{-1}	A	B	C
3^{-1}	1	3	C	A	B
3	3^{-1}	1	B	C	A
A	C	B	1	3^{-1}	3
B	A	C	3	1	3^{-1}
C	B	A	3^{-1}	3	1

In this table the symbols A , B and C , which are elements of order two, stand for the three twofold axes in 32 or for the three planes in $3m$. The group has one sub-group of order three and three sub-groups of order two.

This group is important in group theory in that it is the non-Abelian group of lowest order. Note,

for example, that $AB=3^{-1}$ while $BA=3$, and that $3A=B$ while $A3=C$.

11. The group tables for all the crystallographic groups have not been included in the present edition of these tables. To facilitate the construction of such a table by the reader for any group in which he may have interest, the table for the cubic point group 23 is constructed in detail in Table 2.1.12.3. The matrix representations for the group operations have been used to facilitate this process.

With the aid of this table we can now give a detailed analysis of group 23. It is of order twelve, with three sub-groups of order two and four sub-groups of order three. The operators 2 commute with one another but not with the operators 3, nor do the latter commute with one another.

12. An additional group of great importance to crystallography is the *translation group*. The lattice translations (in three dimensions)

$$n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3$$

(in which the coefficients n_i assume all integral values, positive, negative and zero, and the vectors \mathbf{a}_i are non-coplanar) form an infinite group under the group operation of vector addition and with the zero vector as identity operation.

Some sub-groups of the translation group of interest are constructed as follows.

- (a) Any three non-coplanar translations selected from the group, i.e.

$$\begin{aligned} p_1 \mathbf{a}_1 + p_2 \mathbf{a}_2 + p_3 \mathbf{a}_3 \\ q_1 \mathbf{a}_1 + q_2 \mathbf{a}_2 + q_3 \mathbf{a}_3 \\ r_1 \mathbf{a}_1 + r_2 \mathbf{a}_2 + r_3 \mathbf{a}_3 \end{aligned}$$

generate a translation group which is a sub-group of the original translation group. The determinant

$$D = \begin{vmatrix} p_1 & p_2 & p_3 \\ q_1 & q_2 & q_3 \\ r_1 & r_2 & r_3 \end{vmatrix}$$

has an integral value which is the ratio of the volume of the primitive cell of the sub-group to that of the original translation group. If $D=\pm 1$, the sub-group is the group itself. If $D=\pm n$ (>1), the sub-group is a *superlattice* of the original translation lattice. The sign of D determines the relative "hand" of the two primitive triplets. It is positive if they are both of the same hand and negative if they are of different hands (cf. Vol. I, 2).

- (b) Any translation $p_1 \mathbf{a}_1 + p_2 \mathbf{a}_2 + p_3 \mathbf{a}_3$ selected from the group generates a one-dimensional translation group or *row* (cf. Vol. I, 2) which is a sub-group of the original group. If the coefficients p_i are prime numbers or are relatively prime to one another, then the row is a primitive row of the original lattice. If not, the row is a primitive row of some superlattice of the original lattice.

(c) Any two non-collinear translations, i.e.

$$p_1\mathbf{a}_1 + p_2\mathbf{a}_2 + p_3\mathbf{a}_3$$

$$q_1\mathbf{a}_1 + q_2\mathbf{a}_2 + q_3\mathbf{a}_3$$

generate a two-dimensional translation group or *net* which is a sub-group of the original translation group. If both of the above transla-

tions generate primitive rows of the original lattice and if in addition the three determinants

$$\begin{vmatrix} p_1 p_2 \\ q_1 q_2 \end{vmatrix} \quad \begin{vmatrix} p_1 p_3 \\ q_1 q_3 \end{vmatrix} \quad \begin{vmatrix} p_2 p_3 \\ q_2 q_3 \end{vmatrix}$$

have no common factor except unity, the net is

(Continued on page 33)

TABLE 2.1.12.3
Construction of Group Multiplication Table for the Point Group 23

1	2 _a	2 _b	2 _c	3	3 _a	3 _b	3 _c	3 ⁻¹	3 _b ⁻¹	3 _c ⁻¹	3 _a ⁻¹
2 _a	1	2 _c	2 _b	3 _a	3	3 _c	3 _b	3 _b ⁻¹	3 ⁻¹	3 _a ⁻¹	3 _c ⁻¹
2 _b	2 _c	1	2 _a	3 _b	3 _c	3	3 _a	3 _c ⁻¹	3 _a ⁻¹	3 ⁻¹	3 _b ⁻¹
2 _c	2 _b	2 _a	1	3 _c	3 _b	3 _a	3	3 _a ⁻¹	3 _c ⁻¹	3 _b ⁻¹	3 ⁻¹
3 ⁻¹	3 _a ⁻¹	3 _b ⁻¹	3 _c ⁻¹	1	2 _c	2 _a	2 _b	3	3 _c	3 _a	3 _b
3 _a ⁻¹	3 ⁻¹	3 _c ⁻¹	3 _b ⁻¹	2 _c	1	2 _b	2 _a	3 _c	3	3 _b	3 _a
3 _b ⁻¹	3 _c ⁻¹	3 ⁻¹	3 _a ⁻¹	2 _a	2 _b	1	2 _c	3 _a	3 _b	3	3 _c
3 _c ⁻¹	3 _b ⁻¹	3 _a ⁻¹	3 ⁻¹	2 _b	2 _a	2 _c	1	3 _b	3 _a	3 _c	3
3	3 _b	3 _c	3 _a	3 ⁻¹	3 _c ⁻¹	3 _a ⁻¹	3 _b ⁻¹	1	2 _b	2 _c	2 _a
3 _b	3	3 _a	3 _c	3 _c ⁻¹	3 ⁻¹	3 _b ⁻¹	3 _a ⁻¹	2 _b	1	2 _a	2 _c
3 _c	3 _a	3	3 _b	3 _a ⁻¹	3 _b ⁻¹	3 ⁻¹	3 _c ⁻¹	2 _c	2 _a	1	2 _b
3 _a	3 _c	3 _b	3	3 _b ⁻¹	3 _a ⁻¹	3 _c ⁻¹	3 ⁻¹	2 _a	2 _c	2 _b	1

Notation

(a) The symbol 2_a represents the 2 axis in the *a* direction and it has the matrix representation

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{bmatrix} \text{ etc.}$$

and we have 2_a2_b=2_c, etc.

(b) The symbol 3 represents a positive rotation about the axis [111] and has the pre-factor matrix representation (see 2.4.7.3, p. 63):

$$\begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$

Its inverse 3⁻¹ is, of course,

$$\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$$

(c) The symbol 3_i≡2_i3 and the symbol 3_i⁻¹≡3⁻¹2_i, and the construction of the table then follows directly from the following key results:

$$\left. \begin{aligned} 3_a &\equiv 2_a 3 \equiv \begin{bmatrix} 0 & 0 & 1 \\ \bar{1} & 0 & 0 \\ 0 & \bar{1} & 0 \end{bmatrix} \equiv 3 2_c \\ 3_a^{-1} &\equiv 3^{-1} 2_a \equiv \begin{bmatrix} 0 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \\ 1 & 0 & 0 \end{bmatrix} \equiv 2_c 3^{-1} \end{aligned} \right\} \text{Axis } [\bar{1}1\bar{1}]$$

$$\left. \begin{aligned} 3_b &\equiv 2_b 3 \equiv \begin{bmatrix} 0 & 0 & \bar{1} \\ 1 & 0 & 0 \\ 0 & \bar{1} & 0 \end{bmatrix} \equiv 3 2_a \\ 3_b^{-1} &\equiv 3^{-1} 2_b \equiv \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & \bar{1} \\ \bar{1} & 0 & 0 \end{bmatrix} \equiv 2_a 3^{-1} \end{aligned} \right\} \text{Axis } [\bar{1}\bar{1}1]$$

Notation (continued)

$$\left. \begin{aligned} 3_c &\equiv 2_c 3 \equiv \begin{bmatrix} 0 & 0 & \bar{1} \\ \bar{1} & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \equiv 3 2_b \\ 3_c^{-1} &\equiv 3^{-1} 2_c \equiv \begin{bmatrix} 0 & \bar{1} & 0 \\ 0 & 0 & 1 \\ \bar{1} & 0 & 0 \end{bmatrix} \equiv 2_b 3^{-1} \end{aligned} \right\} \text{Axis } [1\bar{1}\bar{1}]$$

From these key results we can derive many other results, typified by

$$\begin{aligned} 3 3_a &\equiv 3^2 2_c \equiv 3^{-1} 2_c \equiv 3_c^{-1} \\ 3_a 3_b &\equiv 3 2_c 2_b 3 \equiv 3 2_b 2_c 3 \equiv 3_c^2 \equiv 3_c^{-1} \\ 3_a 3_b^{-1} &\equiv 2_a 3^{-1} 2_b \equiv 2_a 2_b \equiv 2_c, \text{ etc.} \end{aligned}$$

(d) Note that the axis for positive rotation 3_a is $[\bar{1}1\bar{1}]$, i.e. the axis which is generated by 2_b from [111]. The operation 2_b does not occur in the definition of 3_a in terms of 3 either as pre-multiplier or post-multiplier. However, 3_a=2_b32_b⁻¹. This latter result is related to the theory of the "transforms" of an operation *Q* by the operation *R*, i.e. *RQR*⁻¹, where *R* is any one of the operations of the group. Such transforms are involved in the theory of "classes," a branch of group theory which is beyond the scope of these notes. For references see [4], [29] and [30].

(e) Note that in the Hermann-Mauguin notation (Vol. I, Section 3.3, Table 3.3.2) for the group 23 a set of twofold axes in the primary directions and a set of threefold axes in the secondary directions is implied. In Table 2.1.12.3 the symbol 23 does not occur, but 2_a3 implies the operation of the axis 3 in the [111] direction followed by a rotation 2 about the *a* direction. The equation 2_a3=32_c does not imply that the space group 23 is equivalent to the space group 32!

a primitive net of the original lattice. If these conditions are not satisfied, the net is a primitive net of some superlattice of the original lattice.

In the space groups, the translation group is always a sub-group.

2.1.12.4. SPACE GROUPS

Space groups in the abstract sense are infinite groups. Each space group of a given crystal class is multiply isomorphous with the point group associated with that class. In this isomorphism all the lattice translations are associated with the identity operation of the point group; all the centres of symmetry (if any) in space are associated with the single centre (if any) in the point group; and all parallel planes of symmetry, rotation axes, or inversion axes, of a given orientation are associated with corresponding planes, rotation or inversion axes of the point group in corresponding orientation, irrespective of the trans-

lational properties of the symmetry element in the space group.

The nature of the above discussion is illustrated by consideration of the general point position for all space groups which are isomorphous with the point group 222 (Table 2.1.12.4). The equivalent positions for this point group are xyz , $x\bar{y}\bar{z}$, $\bar{x}y\bar{z}$, $\bar{x}\bar{y}z$. The equivalent positions for all the space groups are strictly analogous with these positions, the co-ordinates being modified only by the displacements of the axis sets with respect to the origin chosen for a given space group and by the screw components of the axes in question. Each displacement of $\frac{1}{4}$ translation of the axis from the origin adds $\frac{1}{2}$ translation to the corresponding co-ordinate, and each screw component adds itself to the corresponding co-ordinate.

This discussion is somewhat trivial, since it is clear that it is just such considerations which led to the choice of the Hermann-Mauguin symbols and to the arrangement of the space-group tables of Vol. I and of many earlier space-group tables.

TABLE 2.1.12.4
Analysis of General Positions for Space Groups Isomorphous with the Point Group 222

D_2 number	Space Group	Symmetry Elements and Co-ordinates							Lattice Translations
		1	2 · ·		· 2 ·		· · 2		
1	$P222$	xyz	$\begin{smallmatrix} 2 \\ u00 \end{smallmatrix}$	$x\bar{y}\bar{z}$	$\begin{smallmatrix} 2 \\ 0v0 \end{smallmatrix}$	$\bar{x}y\bar{z}$	$\begin{smallmatrix} 2 \\ 00w \end{smallmatrix}$	$\bar{x}\bar{y}z$	
2	$P222_1$	xyz	$\begin{smallmatrix} 2 \\ u00 \end{smallmatrix}$	$x\bar{y}\bar{z}$	$\begin{smallmatrix} 2 \\ 0v\frac{1}{4} \end{smallmatrix}$	$\bar{x}, y, \frac{1}{2}-z$	$\begin{smallmatrix} 2_1 \\ 00w \end{smallmatrix}$	$\bar{x}, \bar{y}, \frac{1}{2}+z$	
3	$P2_12_12$	xyz	$\begin{smallmatrix} 2_1 \\ u\frac{1}{4}0 \end{smallmatrix}$	$\frac{1}{2}+x, \frac{1}{2}-y, \bar{z}$	$\begin{smallmatrix} 2_1 \\ \frac{1}{4}v0 \end{smallmatrix}$	$\frac{1}{2}-x, \frac{1}{2}+y, \bar{z}$	$\begin{smallmatrix} 2 \\ 00w \end{smallmatrix}$	$\bar{x}\bar{y}z$	
4	$P2_12_12_1$	xyz	$\begin{smallmatrix} 2_1 \\ u\frac{1}{4}0 \end{smallmatrix}$	$\frac{1}{2}+x, \frac{1}{2}-y, \bar{z}$	$\begin{smallmatrix} 2_1 \\ 0v\frac{1}{4} \end{smallmatrix}$	$\bar{x}, \frac{1}{2}+y, \frac{1}{2}-z$	$\begin{smallmatrix} 2_1 \\ \frac{1}{4}0w \end{smallmatrix}$	$\frac{1}{2}-x, \bar{y}, \frac{1}{2}+z$	
5	$C222_1$	xyz	$\begin{smallmatrix} 2 \\ u00 \end{smallmatrix}$	$x\bar{y}\bar{z}$	$\begin{smallmatrix} 2 \\ 0v\frac{1}{4} \end{smallmatrix}$	$\bar{x}, y, \frac{1}{2}-z$	$\begin{smallmatrix} 2_1 \\ 00w \end{smallmatrix}$	$\bar{x}, \bar{y}, \frac{1}{2}+z$	$(000; \frac{1}{2}\frac{1}{2}0)+$
6	$C222$	xyz	$\begin{smallmatrix} 2 \\ u00 \end{smallmatrix}$	$x\bar{y}\bar{z}$	$\begin{smallmatrix} 2 \\ 0v0 \end{smallmatrix}$	$\bar{x}y\bar{z}$	$\begin{smallmatrix} 2 \\ 00w \end{smallmatrix}$	$\bar{x}\bar{y}z$	
7	$F222$	xyz	$\begin{smallmatrix} 2 \\ u00 \end{smallmatrix}$	$x\bar{y}\bar{z}$	$\begin{smallmatrix} 2 \\ 0v0 \end{smallmatrix}$	$\bar{x}y\bar{z}$	$\begin{smallmatrix} 2 \\ 00w \end{smallmatrix}$	$\bar{x}\bar{y}z$	$(000; 0\frac{1}{2}\frac{1}{2}; \frac{1}{2}0\frac{1}{2}; \frac{1}{2}\frac{1}{2}0)+$
8	$I222$	xyz	$\begin{smallmatrix} 2 \\ u00 \end{smallmatrix}$	$x\bar{y}\bar{z}$	$\begin{smallmatrix} 2 \\ 0v0 \end{smallmatrix}$	$\bar{x}y\bar{z}$	$\begin{smallmatrix} 2 \\ 00w \end{smallmatrix}$	$\bar{x}\bar{y}z$	$(000; \frac{1}{2}\frac{1}{2}\frac{1}{2})+$
9	$I2_12_12_1$	xyz	$\begin{smallmatrix} 2_1 \\ u\frac{1}{4}0 \end{smallmatrix}$	$\frac{1}{2}+x, \frac{1}{2}-y, \bar{z}$	$\begin{smallmatrix} 2_1 \\ 0v\frac{1}{4} \end{smallmatrix}$	$\bar{x}, \frac{1}{2}+y, \frac{1}{2}-z$	$\begin{smallmatrix} 2_1 \\ \frac{1}{4}0w \end{smallmatrix}$	$\frac{1}{2}-x, \bar{y}, \frac{1}{2}+z$	

It is by no means trivial that similar considerations can greatly facilitate extensions of previous tabulations, as indicated by the example of the next Section.

2.1.12.5. GROUP CONSIDERATIONS AND THE DERIVATION OF VECTOR DISTANCE SETS

In connection with the interpretation of the $|F|^2$ series it is often desirable to calculate the vector distance set for a given set of points which possess the symmetry of a given space group. To clarify the procedure we shall calculate in detail the vectors drawn from the points equivalent to $x_2y_2z_2$ in the space group $P222$ to the points equivalent to $x_1y_1z_1$. This calculation is as follows:

give distance sets with symmetry $Fmmm$ and $Immm$ respectively. For example, the general positions of $Fmmm$ will be occupied four times with exactly the same parameters for $F222$ as for $P222$. These will now be 32-fold positions instead of 8-fold, so that there will be in all 128 general vectors. Similarly, there will be two sets of 64 internal distances, one from each of the sets $x_1y_1z_1$ and $x_2y_2z_2$. Note that there are then 256 vectors within the F -cell, i.e. 4×8^2 . Thus, in this normalization of the vector set each primitive cell of the centred cell is treated separately in forming the vector set.

Reference to Table 2.1.12.4 will indicate directly the form for the vector distances for any other space

	$x_1y_1z_1$	$x_1\bar{y}_1\bar{z}_1$	$\bar{x}_1y_1\bar{z}_1$	$\bar{x}_1\bar{y}_1z_1$
$x_2y_2z_2$	$x_1-x_2, y_1-y_2, z_1-z_2$	$x_1-x_2, \overline{y_1+y_2}, \overline{z_1+z_2}$	$\overline{x_1+x_2}, y_1-y_2, \overline{z_1+z_2}$	$\overline{x_1+x_2}, \overline{y_1+y_2}, z_1-z_2$
$x_2\bar{y}_2\bar{z}_2$	$x_1-x_2, y_1+y_2, z_1+z_2$	$x_1-x_2, \overline{y_1-y_2}, \overline{z_1-z_2}$	$\overline{x_1+x_2}, y_1+y_2, \overline{z_1-z_2}$	$\overline{x_1+x_2}, \overline{y_1-y_2}, z_1+z_2$
$\bar{x}_2y_2\bar{z}_2$	$x_1+x_2, y_1-y_2, z_1+z_2$	$x_1+x_2, \overline{y_1+y_2}, \overline{z_1-z_2}$	$\overline{x_1-x_2}, y_1-y_2, \overline{z_1-z_2}$	$\overline{x_1-x_2}, \overline{y_1+y_2}, z_1+z_2$
$\bar{x}_2\bar{y}_2z_2$	$x_1+x_2, y_1+y_2, z_1-z_2$	$x_1+x_2, \overline{y_1-y_2}, \overline{z_1+z_2}$	$\overline{x_1-x_2}, y_1+y_2, \overline{z_1+z_2}$	$\overline{x_1-x_2}, \overline{y_1-y_2}, z_1-z_2$

If now we remember that the space group of the vector distance set will be $Pmmm$, it is clear that the thirty-two vectors joining $x_1y_1z_1$ and its equivalents with $x_2y_2z_2$ and its equivalents will be expressed in terms of the 8-fold general position 8(a) of the space group $Pmmm$. This will be occupied four times with the four sets of parameters:

$$\begin{aligned} &x_1-x_2, y_1-y_2, z_1-z_2; \quad x_1-x_2, y_1+y_2, z_1+z_2; \\ &x_1+x_2, y_1-y_2, z_1+z_2; \quad x_1+x_2, y_1+y_2, z_1-z_2 \end{aligned}$$

It is clear now that it would only have been necessary to write down the first column of the distance table and that that could have been done by inspection. Setting $x_2=x_1$, etc., we see that the distances between the equivalent points of $x_1y_1z_1$ are, in terms of the equivalent points of $Pmmm$:

4 (a): 000

$$(u): 0, 2y_1, 2z_1; 0, \overline{2y_1}, \overline{2z_1}; 0, \overline{2y_1}, 2z_1; 0, 2y_1, \overline{2z_1}$$

$$(w): 2x_1, 0, 2z_1; \overline{2x_1}, 0, \overline{2z_1}; 2x_1, 0, \overline{2z_1}; \overline{2x_1}, 0, 2z_1$$

$$(y): 2x_1, 2y_1, 0; \overline{2x_1}, \overline{2y_1}, 0; \overline{2x_1}, 2y_1, 0; 2x_1, \overline{2y_1}, 0$$

There is a similar set of points for the internal distances of the set $x_2y_2z_2$.

It should be pointed out here in caution that some "special positions" are required to describe distance sets which are not in fact symmetrical special positions in the sense of the tables of Vol. I.

After this discussion of the space group $P222$, the form taken by the distance sets of the remaining space groups of this class is quite clear. $F222$ and $I222$ will

group of the class. For example, for $P2_12_12$ the general positions of $Pmmm$ will have parameters

$$\begin{aligned} &x_1-x_2, y_1-y_2, z_1-z_2; \frac{1}{2}+x_1-x_2, \frac{1}{2}+y_1+y_2, z_1+z_2; \\ &x_1+x_2, y_1+y_2, z_1-z_2; \frac{1}{2}+x_1+x_2, \frac{1}{2}+y_1-y_2, z_1+z_2; \end{aligned}$$

while the special positions will have parameters $0, 0, 0; 2x_1, 2y_1, 0; \frac{1}{2}, \frac{1}{2}+2y_1, 2z_1; \frac{1}{2}+2x_1, \frac{1}{2}, 2z_1$; etc.

Thus the procedure for determining the vector distances for any space group may be summarized as follows:

1. Form the group table for the point group and its set of equivalent points.
2. Locate the simplest space counterpart of each operation of the point group.
3. Write down the vector components in terms of the general and special positions of the Laue space group.

As a final example to indicate the application of these rules, Table 2.1.12.5 summarizes the discussion for the space group $P2_13$ (cf. Table 2.1.12.3). There are 12 different sets of parameters for the general position of the Laue group $Pm3$, i.e. 288 general vectors. These degenerate as indicated to the 144 special vectors between equivalent atoms.

For references in connection with Section 2.1.12 generally, see [27]–[30]; also [4] and many textbooks on quantum mechanics for discussion of group theory.

2.1. ALGEBRA

TABLE 2.1.12.5

Analysis of Co-ordinates and Vector Distances for the Space Group $P2_13$

Operation	Axis	Location	Co-ordinates	General Vectors $Pm3: 24(l)$	Special Vectors $Pm3$	
1	—	—	x, y, z	$x_1-x_2 \quad y_1-y_2 \quad z_1-z_2$	12(a)	0 0 0
3	1 1 1	0 0 0	z, x, y	$x_1-z_2 \quad y_1-x_2 \quad z_1-y_2$	24(l)	$x-y, y-z, z-x$
3^{-1}	1 1 1	0 0 0	y, z, x	$x_1-y_2 \quad y_1-z_2 \quad z_1-x_2$		
$(2_1)_a$	1 0 0	0 $\frac{1}{4}$ 0	$\frac{1}{2}+x, \frac{1}{2}-y, \bar{z}$	$\frac{1}{2}+x_1-x_2, \frac{1}{2}+y_1+y_2, z_1+z_2$	12(k)	$\frac{1}{2}, \frac{1}{2}+2y, 2z$
3_a	$\bar{1} \ 1 \ \bar{1}$	0 $\frac{1}{2} \ \frac{1}{2}$	$\frac{1}{2}+z, \frac{1}{2}-x, \bar{y}$	$\frac{1}{2}+x_1-z_2, \frac{1}{2}+y_1+x_2, z_1+y_2$	24(l)	$\frac{1}{2}+x+y, y+z, \frac{1}{2}+z-x$
3_a^{-1}	$\bar{1} \ 1 \ \bar{1}$	0 $\frac{1}{2} \ \frac{1}{2}$	$\frac{1}{2}-y, \bar{z}, \frac{1}{2}+x$	$\frac{1}{2}+x_1+y_2, y_1+z_2, \frac{1}{2}+z_1-x_2$		
$(2_1)_b$	0 1 0	0 0 $\frac{1}{4}$	$\bar{x}, \frac{1}{2}+y, \frac{1}{2}-z$	$x_1+x_2, \frac{1}{2}+y_1-y_2, \frac{1}{2}+z_1+z_2$	12(k)	$\frac{1}{2}, \frac{1}{2}+2z, 2x$
3_b	$\bar{1} \ \bar{1} \ 1$	$\frac{1}{2} \ 0 \ \frac{1}{2}$	$\bar{z}, \frac{1}{2}+x, \frac{1}{2}-y$	$x_1+z_2, \frac{1}{2}+y_1-x_2, \frac{1}{2}+z_1+y_2$	24(l)	$\frac{1}{2}+x-y, \frac{1}{2}+y+z, z+x$
3_b^{-1}	$\bar{1} \ \bar{1} \ 1$	$\frac{1}{2} \ 0 \ \frac{1}{2}$	$\frac{1}{2}+y, \frac{1}{2}-z, \bar{x}$	$\frac{1}{2}+x_1-y_2, \frac{1}{2}+y_1+z_2, z_1+x_2$		
$(2_1)_c$	0 0 1	$\frac{1}{4} \ 0 \ 0$	$\frac{1}{2}-x, \bar{y}, \frac{1}{2}+z$	$\frac{1}{2}+x_1+x_2, y_1+y_2, \frac{1}{2}+z_1-z_2$	12(k)	$\frac{1}{2}, \frac{1}{2}+2x, 2y$
3_c	1 $\bar{1} \ \bar{1}$	$\frac{1}{2} \ \frac{1}{2} \ 0$	$\frac{1}{2}-z, \bar{x}, \frac{1}{2}+y$	$\frac{1}{2}+x_1+z_2, y_1+x_2, \frac{1}{2}+z_1-y_2$	24(l)	$x+y, \frac{1}{2}+y-z, \frac{1}{2}+z+x$
3_c^{-1}	1 $\bar{1} \ \bar{1}$	$\frac{1}{2} \ \frac{1}{2} \ 0$	$\bar{y}, \frac{1}{2}+z, \frac{1}{2}-x$	$x_1+y_2, \frac{1}{2}+y_1-z_2, \frac{1}{2}+z_1+x_2$		

2.2. Trigonometry and Geometry

2.2.1. Properties of Trigonometric and Hyperbolic Functions

2.2.1.1. DEFINITIONS

The two fundamental trigonometric quantities are defined by the series

$$\sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \dots = \frac{1}{2i}(e^{ix} - e^{-ix}) \dots (1)$$

and

$$\cos x = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \dots = \frac{1}{2}(e^{ix} + e^{-ix}) \dots (2)$$

The definitions of these functions in terms of the ratios of the sides of a right-angled triangle are

$$\sin A = a/c \dots (3)$$

and

$$\cos A = b/c \dots (4)$$

where the notation is that of Fig. 2.2.1.1 (C is a right angle).

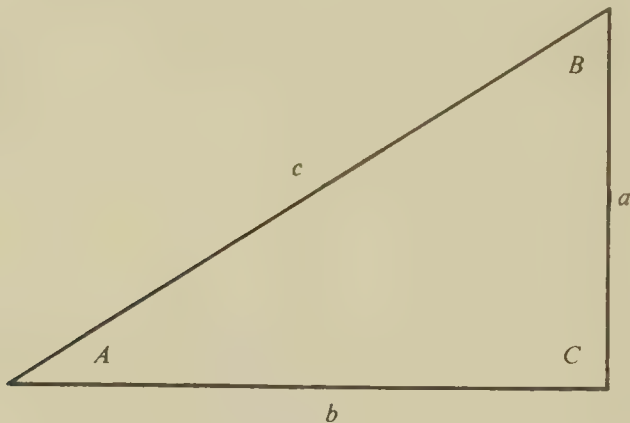


Fig. 2.2.1.1

The definitions (1) and (2) are equivalent respectively to (3) and (4) when the variable x is the radian measure of the corresponding angle.

The functions $\tan x$, $\cot x$, $\sec x$, $\operatorname{cosec} x$ are defined by the equations

$$\tan x = \sin x / \cos x \dots (5)$$

$$\tan x \cdot \cot x = \sin x \cdot \operatorname{cosec} x = \cos x \cdot \sec x = 1 \dots (6)$$

The hyperbolic functions $\sinh x$ and $\cosh x$ are defined by the two series

$$\sinh x = x + \frac{x^3}{3!} + \frac{x^5}{5!} + \frac{x^7}{7!} + \dots = \frac{1}{2}(e^x - e^{-x}) \dots (7)$$

and

$$\cosh x = 1 + \frac{x^2}{2!} + \frac{x^4}{4!} + \frac{x^6}{6!} + \dots = \frac{1}{2}(e^x + e^{-x}) \dots (8)$$

These functions do not have a simple geometric significance. They are related to the trigonometric functions by the relations

$$\sin ix = i \sinh x \dots (9)$$

$$\cos ix = \cosh x \dots (10)$$

with similar definitions for functions $\tanh x$, $\coth x$, $\operatorname{sech} x$, $\operatorname{cosech} x$. Although little further use of hyperbolic functions will be made in these tables, it is worthy of note that, to every relation between trigonometric functions presented in subsequent Sections, there is a corresponding relation between hyperbolic functions which can be established with the aid of (9) and (10).

As a direct consequence of the definitions there result the following fundamental relationships:

$$\sin^2 x + \cos^2 x = 1 \dots (11)$$

$$\operatorname{cosec}^2 x = 1 + \cot^2 x \dots (12)$$

$$\sec^2 x = 1 + \tan^2 x \dots (13)$$

The periodicity of $\sin A$, $\cos A$, and $\tan A$ is as follows:

	$2n\pi \pm A$	$(4n+1)\frac{\pi}{2} \pm A$	$(2n+1)\pi \pm A$	$(4n+3)\frac{\pi}{2} \pm A$
\sin	$\pm \sin A$	$\cos A$	$\mp \sin A$	$-\cos A$
\cos	$\cos A$	$\mp \sin A$	$-\cos A$	$\pm \sin A$
\tan	$\pm \tan A$	$\mp \cot A$	$\pm \tan A$	$\mp \cot A$

Special values for these functions are given in the table below:

	0	$\frac{\pi}{12}$	$\frac{\pi}{6}$	$\frac{\pi}{4}$	$\frac{\pi}{3}$	$\frac{5\pi}{12}$	$\frac{\pi}{2}$
$\sin x$	0	$\frac{\sqrt{3}-1}{2\sqrt{2}}$	$\frac{1}{2}$	$\frac{\sqrt{2}}{2}$	$\frac{\sqrt{3}}{2}$	$\frac{\sqrt{3}+1}{2\sqrt{2}}$	1
$\cos x$	1	$\frac{\sqrt{3}+1}{2\sqrt{2}}$	$\frac{\sqrt{3}}{2}$	$\frac{\sqrt{2}}{2}$	$\frac{1}{2}$	$\frac{\sqrt{3}-1}{2\sqrt{2}}$	0
$\tan x$	0	$2-\sqrt{3}$	$\frac{\sqrt{3}}{3}$	1	$\sqrt{3}$	$2+\sqrt{3}$	∞

2.2.1.2. FUNCTIONS OF MULTIPLE ANGLES

The half-angle formulae are important special cases of multiple-angle formulae.

- (1) $\sin A/2 = \sqrt{\{(1 - \cos A)/2\}}$.
- (2) $\cos A/2 = \sqrt{\{(1 + \cos A)/2\}}$.
- (3) $\tan A/2 = \sqrt{\{(1 - \cos A)/(1 + \cos A)\}}$
 $= (1 - \cos A)/\sin A = \sin A/(1 + \cos A)$.

The general expansions for $\sin nA$ and $\cos nA$ are given by Bromwich [14], Chapter IX. They can be calculated from the binomial expansion

$$\cos nA + i \sin nA = (\cos A + i \sin A)^n$$

- (4) $\sin 2A = 2 \sin A \cos A$.
- (5) $\sin 3A = (4 \cos^2 A - 1) \sin A = (3 - 4 \sin^2 A) \sin A$.
- (6) $\sin 4A = (8 \cos^3 A - 4 \cos A) \sin A$
 $= (4 \sin A - 8 \sin^3 A) \cos A$.
- (7) $\sin 5A = (16 \cos^4 A - 12 \cos^2 A + 1) \sin A$
 $= (5 - 20 \sin^2 A + 16 \sin^4 A) \sin A$.
- (8) $\sin 6A = (32 \cos^5 A - 32 \cos^3 A + 6 \cos A) \sin A$
 $= (6 \sin A - 32 \sin^3 A + 32 \sin^5 A) \cos A$.
- (9) $\cos 2A = \cos^2 A - \sin^2 A = 2 \cos^2 A - 1 = 1 - 2 \sin^2 A$.
- (10) $\cos 3A = 4 \cos^3 A - 3 \cos A = (1 - 4 \sin^2 A) \cos A$.
- (11) $\cos 4A = 8 \cos^4 A - 8 \cos^2 A + 1$
 $= 1 - 8 \sin^2 A + 8 \sin^4 A$.
- (12) $\cos 5A = 16 \cos^5 A - 20 \cos^3 A + 5 \cos A$
 $= (1 - 12 \sin^2 A + 16 \sin^4 A) \cos A$.
- (13) $\cos 6A = 32 \cos^6 A - 48 \cos^4 A + 18 \cos^2 A - 1$
 $= 1 - 18 \sin^2 A + 48 \sin^4 A - 32 \sin^6 A$.

The following are useful special cases of the Fourier series for powers of the trigonometric functions:

- (14) $2 \cos^2 A = 1 + \cos 2A$.
- (15) $4 \cos^3 A = 3 \cos A + \cos 3A$.
- (16) $8 \cos^4 A = 3 + 4 \cos 2A + \cos 4A$.
- (17) $16 \cos^5 A = 10 \cos A + 5 \cos 3A + \cos 5A$.
- (18) $32 \cos^6 A = 10 + 15 \cos 2A + 6 \cos 4A + \cos 6A$.
- (19) $2 \sin^2 A = 1 - \cos 2A$.
- (20) $4 \sin^3 A = 3 \sin A - \sin 3A$.
- (21) $8 \sin^4 A = 3 - 4 \cos 2A + \cos 4A$.
- (22) $16 \sin^5 A = 10 \sin A - 5 \sin 3A + \sin 5A$.
- (23) $32 \sin^6 A = 10 - 15 \cos 2A + 6 \cos 4A - \cos 6A$.

2.2.1.3. ADDITION FORMULAE AND PRODUCT FORMULAE

- (1) $\sin (A \pm B) = \sin A \cos B \pm \cos A \sin B$.
- (2) $\cos (A \pm B) = \cos A \cos B \mp \sin A \sin B$.

Successive applications of the above formulae permit the development of addition formulae for any number of angles, e.g.

- (3) $\sin (A+B+C) = \sin A \cos B \cos C + \cos A \sin B \cos C$
 $+ \cos A \cos B \sin C - \sin A \sin B \sin C$.
- (4) $\cos (A+B+C) = \cos A \cos B \cos C - \cos A \sin B \sin C$
 $- \sin A \cos B \sin C - \sin A \sin B \cos C$.

As direct consequence of the addition formulae, we have the product formulae:

- (5) $2 \sin A \cos B = \sin (A-B) + \sin (A+B)$.
- (6) $2 \cos A \cos B = \cos (A-B) + \cos (A+B)$.

- (7) $2 \sin A \sin B = \cos (A-B) - \cos (A+B)$.
- (8) $4 \cos A \cos B \cos C = \cos (A+B+C)$
 $+ \cos (-A+B+C) + \cos (A-B+C)$
 $+ \cos (A+B-C)$.
- (9) $4 \sin A \sin B \cos C = -\cos (A+B+C)$
 $+ \cos (-A+B+C) + \cos (A-B+C)$
 $- \cos (A+B-C)$.
- (10) $4 \cos A \cos B \sin C = \sin (A+B+C)$
 $+ \sin (-A+B+C) + \sin (A-B+C)$
 $- \sin (A+B-C)$.
- (11) $4 \sin A \sin B \sin C = -\sin (A+B+C)$
 $+ \sin (-A+B+C) + \sin (A-B+C)$
 $+ \sin (A+B-C)$.

Similar formulae for the products of more than three trigonometric functions can be developed from the formulae for the addition of more than three angles.

2.2.1.4. SUMS OF TRIGONOMETRIC FUNCTIONS

- (1) $\sin A \pm \sin B = 2 \sin \frac{1}{2}(A \pm B) \cos \frac{1}{2}(A \mp B)$.
- (2) $\cos A + \cos B = 2 \cos \frac{1}{2}(A+B) \cos \frac{1}{2}(A-B)$.
- (3) $\cos A - \cos B = -2 \sin \frac{1}{2}(A+B) \sin \frac{1}{2}(A-B)$.

The formulae for sums of three and more trigonometric functions are more complicated than those for two, and many forms may be derived from the addition formulae. Typical examples are:

- (4) $\sin A + \sin B + \sin C = \sin (A+B+C)$
 $+ 4 \sin \frac{1}{2}(A+B) \sin \frac{1}{2}(B+C) \sin \frac{1}{2}(C+A)$.
- (5) $-\sin A + \sin B + \sin C = -\sin (A+B+C)$
 $+ 4 \cos \frac{1}{2}(A+B) \sin \frac{1}{2}(B+C) \cos \frac{1}{2}(C+A)$.
- (6) $\cos A + \cos B + \cos C = -\cos (A+B+C)$
 $+ 4 \cos \frac{1}{2}(A+B) \cos \frac{1}{2}(B+C) \cos \frac{1}{2}(C+A)$.
- (7) $-\cos A + \cos B + \cos C = \cos (A+B+C)$
 $+ 4 \sin \frac{1}{2}(A+B) \cos \frac{1}{2}(B+C) \sin \frac{1}{2}(C+A)$.

2.2.1.5. MISCELLANEOUS FORMULAE

Some additional formulae of special interest for the reduction of structure factors are given in Vol. I, page 360.† The following formulae may also be useful.

- (1) $\sin^2 A - \sin^2 B = \cos^2 B - \cos^2 A$
 $= \sin (A+B) \sin (A-B)$.
- (2) $\cos^2 A - \sin^2 B = \cos (A+B) \cos (A-B)$.

Trigonometric functions of a complex variable may be expanded as follows:

- (3) $\sin w = \sin (x+iy) = \sin x \cos iy + \cos x \sin iy$
 $= \sin x \cosh y + i \cos x \sinh y$.
- (4) $\cos w = \cos (x+iy) = \cos x \cos iy - \sin x \sin iy$
 $= \cos x \cosh y - i \sin x \sinh y$.

† Note by General Editor. There is a misprint on page 360 of Volume I.

$$\begin{aligned} \sin A + \sin B + \sin C + \sin (A+B-C) \\ = 4 \sin \frac{A+B}{2} \sin \frac{C-A}{2} \sin \frac{C-B}{2} \\ \text{should be } 4 \sin \frac{A+B}{2} \cos \frac{C-A}{2} \cos \frac{C-B}{2} \end{aligned}$$

The correct formula was applied in simplifying structure-factor formulae.

2.2.1.6. APPROXIMATIONS FOR TRIGONOMETRIC FUNCTIONS

It is often necessary to replace one trigonometric function by another or by an algebraic expression in a range in which both have approximately the same value. Frequently used approximate relations (valid for small x) are, in order of decreasing range:

- (1) $\sin x \approx x - x^3/6$.
- (2) $\cos x \approx 1 - x^2/2$.
- (3) $\sin x \approx x$.
- (4) $\tan x \approx x$.
- (5) $\tan x \approx \sin x$.

Table 2.2.1.6A indicates the ranges in which these relations hold within defined accuracy limits.

2.2.1.6.1. *Least Squares Approximations*

Addition of further terms to the defining series for the trigonometric functions will, of course, give increased accuracy of approximation, but this procedure has great disadvantages from a practical point of view, since these series give high accuracy near $x=0$ and concentrate their largest errors near the end of the range in which they are used. If an approximation is required over a definite range, between A and $A+a$, it is more efficient to use a series such as

$$\cos(A+x) \approx C_0 + C_1x + C_2x^2 \quad \dots (1)$$

in which the constants are chosen to give the best fit for the given range by least squares methods (see Section

TABLE 2.2.1.6A
Ranges for Approximations for Trigonometric Functions

The integers in braces in columns 8–12 indicate the largest value of x (to three decimal places) for which the exact values of the function and of the approximation agree to less than one unit in the specified decimal place. Thus {3} in column 11 for $x=0.143$ indicates $\tan x - x = 0.143983 - 0.143000 = 0.000983$, i.e. less than one unit in the third place. It is then implied by the table that for $x=0.144$, $\tan x - x = 0.145004 - 0.144000 = 0.001004$ is greater than or equal to one unit in the

third place. If both the approximation and the function are rounded to the specified number of decimal places the specified difference may occur for lower values of x . The entry in column 1 gives the angle in degrees (to two decimal places) corresponding to x radians, while the entries in columns 2, 3, 5, 6 and 7 give the values to 5 decimal places of the trigonometric functions and their approximations at the critical values of x .

1	2	3	4	5	6	7	8	9	10	11	12
Degrees	$x - x^3/6$	$\sin x$	x	$\tan x$	$1 - x^2/2$	$\cos x$	$\sin x \approx x - x^3/6$	$\cos x \approx 1 - x^2/2$	$\sin x \approx x$	$\tan x \approx x$	$\tan x \approx \sin x$
3.32	.05797	.05797	.058	.05807	.99832	.99832					{4}
3.78	.06595	.06595	.066	.06610	.99782	.99782				{4}	
4.81	.08390	.08390	.084	.08420	.99647	.99647			{4}		
7.16	.12467	.12467	.125	.12566	.99219	.99220					{3}
8.19	.14251	.14251	.143	.14398	.98978	.98979				{3}	
10.37	.18001	.18001	.181	.18300	.98362	.98366			{3}		
12.66	.21920	.21921	.221	.22467	.97558	.97568		{4}			
15.41	.26576	.26577	.269	.27568	.96382	.96404					{2}
17.53	.30122	.30125	.306	.31592	.95318	.95355				{2}	
22.46	.38196	.38204	.392	.41339	.92317	.92415			{2}		
22.57	.38381	.38389	.394	.41574	.92238	.92338		{3}			
23.66	.40126	.40136	.413	.43820	.91472	.91592	{4}				
32.49	.53662	.53710	.567	.63674	.83926	.84352					{1}
36.15	.58913	.58995	.631	.73065	.80092	.80744				{1}	
37.53	.60816	.60916	.655	.76812	.78549	.79305	{3}				
40.22	.64434	.64575	.702	.84571	.75360	.76355		{2}			
48.87	.74956	.75326	.853	1.15	.63620	.65773			{1}		
59.70	.85344	.86341	1.042	1.71	.45712	.50449	{2}				
72.25	.92681	.95240	1.261	3.12	.20494	.30486		{1}			
95.45	.99532	.99547	1.666	-10.47	-.38778	-.09506	{1}				

2.6.6.4, page 92). The constants are solutions of the normal equations

$$I_0C_0 + I_1C_1 + I_2C_2 = J_0$$

$$I_1C_0 + I_2C_1 + I_3C_2 = J_1$$

$$I_2C_0 + I_3C_1 + I_4C_2 = J_2$$

and the total squared departure over the range is E_2 , given by

$$E_2 = K_0 - C_0J_0 - C_1J_1 - C_2J_2 \quad \dots (2)$$

where $K_0 = \int_0^a \cos^2(A+x)dx$,

$$I_n = \int_0^a x^n dx, \text{ and } J_n = \int_0^a x^n \cos(A+x)dx.$$

It is difficult to estimate the maximum departure of such an approximation, but the mean squared error is of course given by $E_2/I_0 = E_2/a$. An example of the use of a series of the type (1) in machine computation of cosines for structure factors is given in Table 2.2.1.6B.

TABLE 2.2.1.6B

Series for Linear Interpolation for Cosine

Explanation. The cosine of the argument x (quadrants) is to be approximated by the series

$$\cos \pi x/2 = C_0 + C_1|x-A|$$

The range is divided into 20 sub-ranges above and below the values $A=0.05(2r+1)$ for $r=0, 1, \dots, 9$. The greatest departure of the rounded-up approximation is one unit in the third place. With obvious modifications the same numbers enter into the calculation of

$$\sin \pi x/2 = S_0 + S_1|x-A|$$

A	C ₀	C ₁	
		x > A	x < A
0.05	0.9974	-0.1846	0.0617
0.15	0.9729	-0.4263	0.3064
0.25	0.9244	-0.6573	0.5436
0.35	0.8531	-0.8726	0.7674
0.45	0.7608	-1.0661	0.9723
0.55	0.6498	-1.2334	1.1533
0.65	0.5228	-1.3703	1.3059
0.75	0.3829	-1.4735	1.4263
0.85	0.2336	-1.5404	1.5116
0.95	0.0785	-1.5694	1.5597

2.2.1.6.2. Approximations for Sketching

In making rough sketches on squared paper it is useful to know that in many cases a simple rational fraction will give a close approximation to the tangent of an angle which occurs frequently. For example, in drawing hexagonal nets on squared paper one may use the ratios 7/4, 12/7, 19/11 as tangents of angles which lie within 15' of 60°. For the tetrahedral angle (109° 28') the fractions 14/5, 17/6, 20/7, 23/8, 25/9, 31/11 give tangent approximations which are within 20' of the correct angle. For the half-tetrahedral angle the useful approximations to the tangent are 7/5, 10/7, 17/12, all of which are within 20' of the correct angle.

2.2.2. Plane Trigonometry

2.2.2.1. NOTATION

The sides and angles of a plane triangle are given by the notation of Fig. 2.2.2.1. The perimeter $2s=a+b+c$, the area of the triangle is S . The centre of the inscribed circle (radius r) lies on the intersection of the bisectors of the vertex angles and is always inside the triangle. The centre of the circumscribed circle (radius R) lies on the intersection of the perpendicular bisectors of the sides. It lies outside the triangle if one of the angles is obtuse.

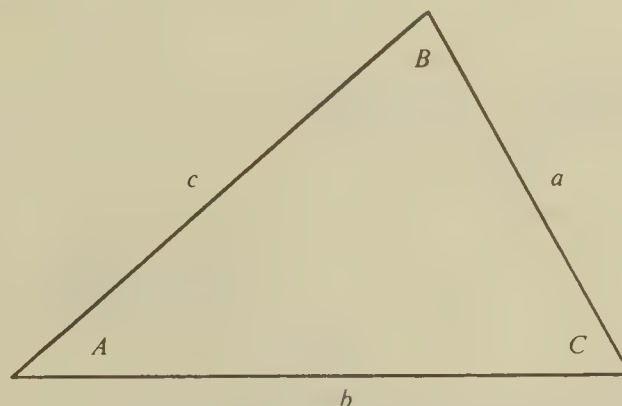


Fig. 2.2.2.1

2.2.2.2. BASIC FORMULAE AND PROPERTIES

- (1) $a/\sin A = b/\sin B = c/\sin C = 2R$.
- (2) $a^2 = b^2 + c^2 - 2bc \cos A$, etc.
- (3) $A + B + C = \pi$.

A plane triangle is determined uniquely by (i) three sides, (ii) two angles and one side, (iii) two sides and the included angle. There are two solutions in general if (iv) two sides and one non-included angle are given. If (v) three or two angles are given, there are infinitely many similar triangles which have these angles, and in them any two of the sides are determined in terms of the third.

Any three lengths can form the sides of a plane triangle if, and only if, the sum of the lengths of any two sides is greater than that of the third.

All problems connected with the complete solution of a plane triangle can be solved in terms of (1), (2),

and (3) above. In special cases, however, there are countless other derivative results of plane trigonometry which will lead to an answer more rapidly than do these formulae.

2.2.2.3. SPECIAL PROPERTIES OF THE PLANE TRIANGLE

- (1) $S = \frac{1}{2}bc \sin A$, etc.
- (2) $S^2 = s(s-a)(s-b)(s-c)$.
- (3) $S = \frac{1}{2}a^2 \sin B \sin C / \sin A$, etc.
- (4) $S = abc/4R$.
- (5) $S = rs$.
- (6) $\sin^2 A/2 = (s-b)(s-c)/bc$, etc.
- (7) $\cos^2 A/2 = s(s-a)/bc$, etc.
- (8) $r = (s-a) \tan \frac{1}{2}A$, etc.

2.2.2.4. REGULAR CONVEX POLYGONS, n SIDES

R = radius of circumscribed circle.

r = radius of inscribed circle.

Angle subtended at centre by one side = $2\pi/n$.

Exterior angle between sides = $\pi + 2\pi/n$.

Interior angle between sides = $\pi - 2\pi/n$.

Length of sides = $L = 2R \sin \pi/n$.

Radius of inscribed circle = $r = R \cos \pi/n$.

Area of polygon = $n r L / 2 = \frac{1}{2} n R^2 \sin 2\pi/n$.

Perimeter = $2nR \sin \pi/n$.

2.2.3. Spherical Trigonometry

2.2.3.1. NOTATION

In a spherical triangle the sides are great circles on the surface of a sphere (radius R). The measures of the sides a, b, c are the angles subtended by the corresponding great circle at the centre of the sphere. The angles A, B, C are the angles between the planes (passing through the centre of the sphere) which contain the sides of the spherical triangle.

It is a common convention to consider only those spherical triangles whose sides and angles are less than π . The properties of all more general spherical triangles can be deduced from these.

2.2.3.2. BASIC FORMULAE

- (1) $\frac{\sin A}{\sin a} = \frac{\sin B}{\sin b} = \frac{\sin C}{\sin c}$.
- (2) $\cos a = \cos b \cos c + \sin b \sin c \cos A$, etc.
- (3) $\cos A = -\cos B \cos C + \sin B \sin C \cos a$, etc.
- (4) $\pi < A + B + C < 3\pi$.

A spherical triangle is determined uniquely by (i) three sides, (ii) three angles, (iii) two sides and their included angle, and (iv) one side and the two adjacent angles. There may be two solutions if (v) two sides and one non-included angle are given, or if (vi) two angles and one non-included side are given.

As in the case of plane trigonometry, all problems

in spherical trigonometry can be solved by means of the above fundamental formulae.

2.2.3.3. POLAR TRIANGLES

Poles of the great circles which form the sides of the spherical triangle ABC define the vertices of the *polar triangle* $A'B'C'$. A' is chosen as that pole of the great circle BC which lies on the same side of it as does A , and a similar convention is adopted in the choice of B' and C' . The following relations then hold:

- (1) If $A'B'C'$ is the polar triangle of ABC , the converse is also true.
- (2) $A = \pi - a'$, $B = \pi - b'$, $C = \pi - c'$.
 $A' = \pi - a$, $B' = \pi - b$, $C' = \pi - c$.

2.2.3.4. RIGHT-ANGLED SPHERICAL TRIANGLES

There are ten formulae connecting the sides a, b, c and the angles A, B of a triangle in which the angle C is a right angle which may be derived from the basic relations 2.2.3.2(1)–(3). These are:

- (1) $\cos c = \cos a \cos b$.
- (2) $\cos c = \cot A \cot B$.
- (3) $\sin a = \sin c \sin A$.
- (4) $\sin b = \sin c \sin B$.
- (5) $\tan a = \tan c \cos B$.
- (6) $\tan b = \tan c \cos A$.
- (7) $\tan a = \sin b \tan A$.
- (8) $\tan b = \sin a \tan B$.
- (9) $\cos B = \cos b \sin A$.
- (10) $\cos A = \cos a \sin B$.

All of these formulae can be remembered by means of the diagram of Fig. 2.2.3.4(1) and the mnemonic known as Napier's Rules. The circle is divided into five parts by radii as shown, and the unique radius is labelled $C (=90^\circ)$. The remaining five sides and angles are placed round the circle in order, the complements

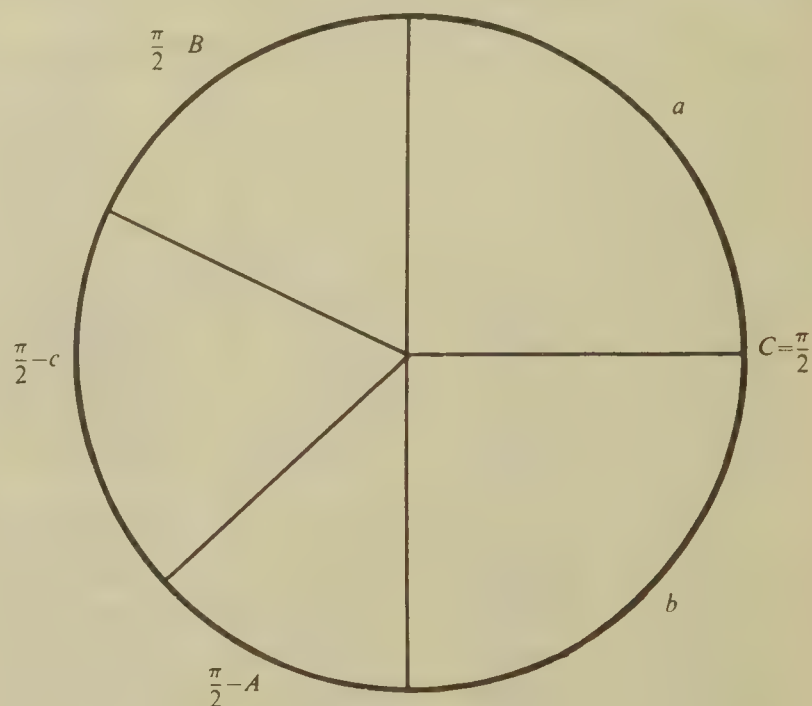


Fig. 2.2.3.4(1)

of the side and angles not adjacent to C being taken. Napier's Rules then may be remembered as:

- (a) sIn mIddle equals tAngents AdjAcent.
(b) sIn mIddle equals cOsines OppOsite.

As for example:

$$\sin \left(\frac{\pi}{2} - A \right) = \tan \left(\frac{\pi}{2} - c \right) \tan b, \text{ i.e. } \tan b = \tan c \cos A \quad \dots (6)$$

$$\sin \left(\frac{\pi}{2} - c \right) = \cos a \cos b, \text{ i.e. } \cos c = \cos a \cos b \dots (I)$$

If the side c is a right angle there are again ten relations between the remaining sides and angles, which may be obtained by considering the polar triangle of that triangle used in deriving (1)–(10) above and by dropping the primes.

- (11) $\cos C = -\cos A \cos B.$
- (12) $\cos C = -\cot a \cot b.$
- (13) $\sin A = \sin C \sin a.$
- (14) $\sin B = \sin C \sin b.$
- (15) $\tan A = -\tan C \cos b.$
- (16) $\tan B = -\tan C \cos a.$
- (17) $\tan A = \sin B \tan a.$
- (18) $\tan B = \sin A \tan b.$
- (19) $\cos b = \cos B \sin a.$
- (20) $\cos a = \cos A \sin b.$

These results can, of course, be written down directly from Napier's Rules after substituting the polar angles in the diagram of Fig. 2.2.3.4(1) or, alternatively, by using the diagram of Fig. 2.2.3.4(2).

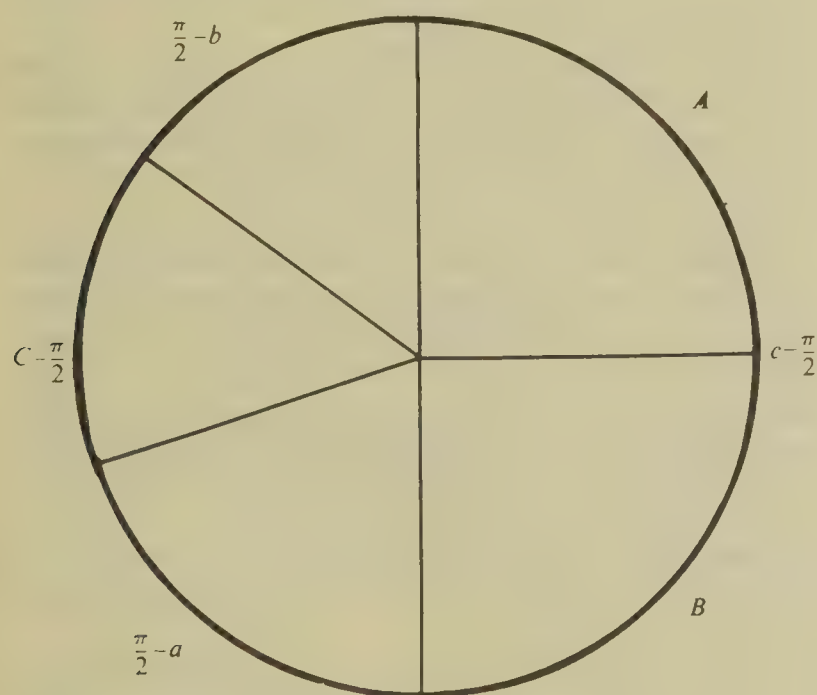


Fig. 2.2.3.4(2)

2.2.3.5. SOLID ANGLE

The surface area of a sphere of radius R is $4\pi R^2$. The unit of solid angle (the solid radian or steradian) is defined as the solid angle subtended at the centre of a sphere of unit radius by unit area on the surface of the sphere. Thus, the total solid angle subtended at a point by any surface which completely encloses that

point is 4π . The *spherical degree* is defined as the solid angle subtended at the centre of a sphere by a spherical triangle having two equal right-angled sides and a vertex angle of 1° . Thus, the solid angle subtended by the whole sphere at the centre is 720 spherical degrees. The ratio of the spherical degree to the steradian is the same as the ratio of the angular degree to the angular radian, i.e. $4\pi/720 = 2\pi/360 = \pi/180$.

The *spherical excess* E of a spherical triangle is defined as the difference between the sum of the angles of the spherical triangle and two right angles.

The area \mathcal{L} of any spherical triangle in spherical measure is equal to the spherical excess in angular measure. We have the three fundamental results

$$E=A+B+C-\pi \quad \dots (1)$$

$$\Sigma = E \quad \dots\dots(2)$$

$$S = \Sigma R^2 = ER^2 \quad \dots\dots(3)$$

where S is the surface area of the spherical triangle in square measure and all spherical and angular measures are in radians.

Textbooks on spherical trigonometry, crystal measurement, spherical astronomy and navigation carry formulae which may be of interest. A text specially adapted to those familiar with crystallographic techniques is given as reference [31].

2.2.4. Plane Analytic Geometry

The results of this section apply to Cartesian coordinates only, except where noted. The results for oblique systems are best expressed in vector or tensor notation (see Section 2.4, page 52).

2.2.4.1. STRAIGHT LINE

(a) Intercept Equation

$$x/a + y/b = 1 \quad \dots\dots(1)$$

where a, b are the intercepts on the x and y axes respectively. Valid also for oblique axes.

(b) Slope and Intercept Equation

$$y=qx+b \quad \dots\dots(2)$$

where $q = -b/a$ is the tangent of the angle which the line makes with the axis of x , and b is the intercept on the y axis.

(c) Perpendicular Equation

$$lx+my-p=0 \quad \dots\dots(3a)$$

$$l^2 + m^2 = 1 \quad \dots\dots(3b)$$

where p is a positive number equal to the length of the perpendicular from the origin on to the line, and l and m are the cosines of the angles which this perpendicular makes with the positive axes of x and y respectively.

(d) *Line through Two Points*

The straight line through two points in Cartesian or oblique systems is

$$(x-x_1)/(x_2-x_1)=(y-y_1)/(y_2-y_1) \quad \dots\dots(4)$$

(e) *General Equation*

The general equation for a straight line is

$$Ax + By + C = 0 \quad \dots (5)$$

This can be reduced to the special forms (1)–(3) above by the relations which follow:

$$a = -C/A, b = -C/B, q = -A/B \quad \dots (6)$$

and if s is the sign of C in (5) and the positive value of the root is taken:

$$l = -sA/\sqrt{(A^2 + B^2)}, \quad m = -sB/\sqrt{(A^2 + B^2)}, \\ p = sC/\sqrt{(A^2 + B^2)} \quad \dots (7)$$

(f) *Perpendicular Distance from a Point on to a Line*

$$P = lx_1 + my_1 - p \quad \dots (8)$$

is the distance from the point x_1y_1 to the line (3a). It is positive if x_1y_1 is on the side of the line opposite to that containing the origin.

(g) *Intersection of Two Lines*

The two lines

$$\begin{cases} A_1x + B_1y + C_1 = 0 \\ A_2x + B_2y + C_2 = 0 \end{cases} \quad \dots (9)$$

intersect in the point (x_0y_0) , which is the solution of these two equations simultaneously, i.e.

$$\begin{aligned} x_0 &= (B_1C_2 - B_2C_1)/(A_1B_2 - A_2B_1) \\ y_0 &= (A_2C_1 - A_1C_2)/(A_1B_2 - A_2B_1) \end{aligned} \quad \dots (10)$$

If the two equations are reduced to the form (3a), i.e.

$$\begin{cases} l_1x + m_1y - p_1 = 0 \\ l_2x + m_2y - p_2 = 0 \end{cases} \quad \dots (11)$$

the solution is:

$$\begin{aligned} x &= (p_1m_2 - p_2m_1)/(l_1m_2 - l_2m_1) \\ y &= (l_1p_2 - l_2p_1)/(l_1m_2 - l_2m_1) \end{aligned} \quad \dots (12)$$

The angle α between the two lines is the angle between their normals, which is given by

$$\cos \alpha = l_1l_2 + m_1m_2 \quad \dots (13)$$

Thus if

$$l_1l_2 + m_1m_2 = 0 \quad \dots (14)$$

the two lines are at right angles. If

$$l_1l_2 + m_1m_2 = \pm 1 \quad \dots (15a)$$

or equivalently

$$l_1m_2 - l_2m_1 = 0 \quad \dots (15b)$$

or

$$A_1B_2 - A_2B_1 = 0 \quad \dots (15c)$$

the two lines are parallel.

(h) *Area of a Triangle of Given Vertices*

The area Δ of a triangle with vertices x_iy_i is

$$\Delta = \pm \frac{1}{2} \begin{vmatrix} x_1y_1 & 1 \\ x_2y_2 & 1 \\ x_3y_3 & 1 \end{vmatrix} \quad \dots (16)$$

the sign being chosen to make the area positive.

2.2.4.2. CURVES OF THE SECOND DEGREE

Any plane curve of the second degree is a conic section and can be reduced to one of nine standard forms as indicated in Table 2.2.4.2.

TABLE 2.2.4.2

Reduction of General Quadratic

$$a_{11}x_1^2 + a_{22}x_2^2 + 2a_{12}x_1x_2 + 2a_{31}x_1 + 2a_{32}x_2 + a_{33} = 0 \quad \dots (17)$$

$$S = \begin{vmatrix} a_{11} & a_{12} & a_{31} \\ a_{12} & a_{22} & a_{32} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} \quad D = \begin{vmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \end{vmatrix}$$

Reduction to centre ($D \neq 0$)

The co-ordinates α_i of the centre are given by

$$D\alpha_1 = -a_{31}a_{22} + a_{32}a_{12} \quad \dots (18a)$$

$$D\alpha_2 = a_{31}a_{12} - a_{32}a_{11} \quad \dots (18b)$$

The substitution

$$x_i = w_i + \alpha_i$$

then leads to

$$a_{11}w_1^2 + a_{22}w_2^2 + 2a_{12}w_1w_2 + S/D = 0 \quad \dots (19)$$

Reduction to Principal Axes

The quadratic terms in (17) or (19) can be reduced to a sum of squares by the methods of 2.1.8.6. Literal methods are given in many texts on analytic geometry, but in numerical examples the matrix approach is usually simpler.

NOTE. When \pm signs are shown, corresponding signs must be taken throughout. Thus in entry (1) below, λ_1 and λ_2 must be both plus or both minus and S must have the opposite sign. In entry (7), λ_1 and δ must have opposite signs. When the two roots are opposite in sign we have arbitrarily chosen λ_1 to be positive.

TABLE 2.2.4.2 (continued). CASE I. $D \neq 0$.

Transform to centre and to principal axes: $\lambda_1y_1^2 + \lambda_2y_2^2 + S/D = 0$

	λ_1	λ_2	D	S	Standard Form	Conic	Special Cases
1	\pm	\pm	+	\mp	$X^2/A^2 + Y^2/B^2 = 1$	Ellipse	Circle
2	\pm	\pm	+	\pm	$X^2/A^2 + Y^2/B^2 = -1$	Imaginary ellipse	Imaginary circle
3	+	-	-	\pm	$X^2/A^2 - Y^2/B^2 = 1$	Hyperbola	
4	+	-	-	0	$X^2/A^2 - Y^2/B^2 = 0$	Pair of intersecting real lines	
5	\pm	\pm	+	0	$X^2/A^2 + Y^2/B^2 = 0$	Pair of imaginary lines with real intersection	

(Continued on next page)

TABLE 2.2.4.2 (continued)

CASE II. $D=0$; $\lambda_2=0$.Transform to principal axes: $\lambda_1 y_1^2 + 2\nu_1 y_1 + 2\nu_2 y_2 + a_{33} = 0$.Remove linear term in y_1 by completing squares: $\lambda_1 z_1^2 + 2\nu_2 y_2 + \delta = 0$.

	λ_1	ν_2	δ	Standard Form	Conic	Remarks
6	$\neq 0$	$\neq 0$	\pm	$Y^2 = 4AX$	Parabola	Remove constant term by shift of origin
7	\pm	0	\mp	$X^2 = A^2$	Pair of real parallel lines	
8	\pm	0	\pm	$X^2 = -A^2$	Pair of imaginary parallel lines	
9	$\neq 0$	0	0	$X^2 = 0$	Pair of coincident lines	

2.2.4.3. GENERAL PROPERTIES OF PLANE CURVES

In general, a real straight line intersects a real curve of the n th degree in n points.

If the equation of the curve is given in the form

$$y = \phi(x)$$

and x_0, y_0 be a point on the curve, the tangent to the curve at x_0, y_0 will be the line

$$\frac{y - y_0}{x - x_0} = \left(\frac{dy}{dx} \right)_0$$

If the equation of the curve is expressed in the form

$$\psi(x, y) = 0$$

the equation of the tangent at the point (x_0, y_0) will be

$$(x - x_0) \left(\frac{\partial \psi}{\partial x} \right)_0 + (y - y_0) \left(\frac{\partial \psi}{\partial y} \right)_0 = 0$$

The radius of curvature ρ of a plane curve is given by

$$\frac{1}{\rho} = \frac{d^2 y / dx^2}{\left\{ 1 + \left(\frac{dy}{dx} \right)^2 \right\}^{3/2}}$$

2.2.5. Solid Analytic Geometry

The results of this section apply in general only to Cartesian co-ordinates except where noted. The results for oblique systems are best expressed in vector or tensor notation.

2.2.5.1. THE PLANE

(a) Intercept Equation

$$x/a + y/b + z/c = 1 \quad \dots (1)$$

where a, b, c are the intercepts on the x, y, z axes respectively. Valid also for oblique axes.

(b) Perpendicular Equation

$$lx + my + nz - p = 0 \quad \dots (2a)$$

$$l^2 + m^2 + n^2 = 1 \quad \dots (2b)$$

where p is a positive number equal to the length of the perpendicular from the origin on to the plane, and l, m, n are the cosines of the angles which this line makes with the positive x, y, z axes respectively.

(c) Plane through Three Points

The equation of the plane through three points $x_i y_i z_i$ is given by the determinant

$$\begin{vmatrix} x & y & z & 1 \\ x_1 & y_1 & z_1 & 1 \\ x_2 & y_2 & z_2 & 1 \\ x_3 & y_3 & z_3 & 1 \end{vmatrix} = 0 \quad \dots (3)$$

(d) The General Equation

The general equation for the plane

$$Ax + By + Cz + D = 0 \quad \dots (4)$$

can be reduced to the special forms (1) and (2) by the following relations:

$$a = -D/A, \quad b = -D/B, \quad c = -D/C \quad \dots (5)$$

and if s is the sign of D in (4) and the positive value of the root is taken:

$$\begin{aligned} l &= -sA/\sqrt{(A^2 + B^2 + C^2)}, \quad m = -sB/\sqrt{(A^2 + B^2 + C^2)}, \\ n &= -sC/\sqrt{(A^2 + B^2 + C^2)} \\ \text{and} \quad p &= sD/\sqrt{(A^2 + B^2 + C^2)} \quad \dots (6) \end{aligned}$$

(e) Perpendicular Distance from a Point on to a Plane

$$P = lx_1 + my_1 + nz_1 - p \quad \dots (7)$$

is the distance from the point $x_1 y_1 z_1$ to the plane (2a). It is positive if the point $(x_1 y_1 z_1)$ is on the side of the plane opposite to that containing the origin.

(f) Angle between Two Planes

The planes

$$\begin{cases} l_1 x + m_1 y + n_1 z - p_1 = 0 \\ l_2 x + m_2 y + n_2 z - p_2 = 0 \end{cases} \quad \dots (8)$$

intersect at an angle θ given by the angle between their outward normals, i.e.

$$\cos \theta = l_1 l_2 + m_1 m_2 + n_1 n_2 \quad \dots (9a)$$

The planes are parallel if

$$l_1 l_2 + m_1 m_2 + n_1 n_2 = \pm 1 \quad \dots (9b)$$

and they intersect at right angles if

$$l_1 l_2 + m_1 m_2 + n_1 n_2 = 0 \quad \dots (9c)$$

2.2.5.2. THE LINE

The specification of a line in three dimensions involves two linear equations, i.e. the equations of any two planes which intersect in the line (cf. (8) above).

(a) Line through Two Points

$$(x-x_1)/(x_2-x_1) = (y-y_1)/(y_2-y_1) = (z-z_1)/(z_2-z_1) \quad \dots (10)$$

(b) Line through One Point in a Given Direction

$$(x-x_1)/\lambda = (y-y_1)/\mu = (z-z_1)/\nu \quad \dots (11)$$

is a line through $x_1 y_1 z_1$ in a direction given by $\lambda \mu \nu$, which are *proportional* to the direction cosines lmn of the line. If $\lambda^2 + \mu^2 + \nu^2 = 1$, λ, μ, ν are in fact the direction cosines of the line.

(c) The General Equation for a Line

The two planes

$$\begin{cases} A_1 x + B_1 y + C_1 z + D_1 = 0 \\ A_2 x + B_2 y + C_2 z + D_2 = 0 \end{cases} \quad \dots (12)$$

define a line whose direction cosines are proportional to λ, μ, ν given by

$$\lambda = B_1 C_2 - B_2 C_1, \quad \mu = C_1 A_2 - C_2 A_1, \quad \nu = A_1 B_2 - A_2 B_1 \quad \dots (13)$$

and one form for the equation of this line is

$$\frac{x - (B_1 D_2 - B_2 D_1)/\nu}{\lambda} = \frac{y + (A_1 D_2 - A_2 D_1)/\nu}{\mu} = \frac{z}{\nu} \quad \dots (14)$$

(d) Properties of Two Lines

Consider the lines

$$\begin{cases} (x-x_1)/l_1 = (y-y_1)/m_1 = (z-z_1)/n_1 \\ (x-x_2)/l_2 = (y-y_2)/m_2 = (z-z_2)/n_2 \end{cases} \quad \dots (15)$$

where $l_1 m_1 n_1$, etc., are direction cosines.

The shortest distance between the two lines is given by

$$\left| \begin{matrix} (x_1-x_2) & (y_1-y_2) & (z_1-z_2) \\ l_1 & m_1 & n_1 \\ l_2 & m_2 & n_2 \end{matrix} \right| \div \sqrt{(\lambda^2 + \mu^2 + \nu^2)} \quad \dots (16)$$

and the direction cosines of this shortest line are proportional to λ, μ, ν , given by

$$\frac{\lambda}{(m_1 n_2 - m_2 n_1)} = \frac{\mu}{(n_1 l_2 - n_2 l_1)} = \frac{\nu}{(l_1 m_2 - l_2 m_1)} \quad \dots (17)$$

The condition that the two lines be coplanar is then that

$$\left| \begin{matrix} (x_1-x_2) & (y_1-y_2) & (z_1-z_2) \\ l_1 & m_1 & n_1 \\ l_2 & m_2 & n_2 \end{matrix} \right| = 0 \quad \dots (18)$$

and the equation for the common plane is

$$\left| \begin{matrix} x-x_1 & y-y_1 & z-z_1 \\ l_1 & m_1 & n_1 \\ l_2 & m_2 & n_2 \end{matrix} \right| = 0 \quad \dots (19)$$

(e) Volume of a Tetrahedron

The volume V of a tetrahedron whose vertices are $x_i y_i z_i$ is given by

$$6V = \pm \begin{vmatrix} x_1 & y_1 & z_1 & 1 \\ x_2 & y_2 & z_2 & 1 \\ x_3 & y_3 & z_3 & 1 \\ x_4 & y_4 & z_4 & 1 \end{vmatrix} \quad \dots (20)$$

2.2.5.3. SURFACES OF THE SECOND DEGREE

An analysis of the general equation of the second degree is given in Table 2.2.5.3, together with the standard forms for the 16 types of surfaces which can arise.

TABLE 2.2.5.3

Reduction of General Conicoid

$$a_{11}x_1^2 + a_{22}x_2^2 + a_{33}x_3^2 + 2a_{12}x_1x_2 + 2a_{23}x_2x_3 + 2a_{31}x_3x_1 + 2a_{41}x_1 + 2a_{42}x_2 + 2a_{43}x_3 + a_{44} = 0 \quad \dots (21)$$

$$S = \begin{vmatrix} a_{11} & a_{12} & a_{31} & a_{41} \\ a_{12} & a_{22} & a_{23} & a_{42} \\ a_{31} & a_{23} & a_{33} & a_{43} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{vmatrix}$$

$$D = \begin{vmatrix} a_{11} & a_{12} & a_{31} \\ a_{12} & a_{22} & a_{23} \\ a_{31} & a_{23} & a_{33} \end{vmatrix}$$

Reduction to Centre ($D \neq 0$)

The co-ordinates α_i of the centre are given by $\alpha_1 = -(a_{41}A_{11} + a_{42}A_{12} + a_{43}A_{31})/D$

$$\alpha_2 = -(a_{41}A_{12} + a_{42}A_{22} + a_{43}A_{23})/D$$

$$\alpha_3 = -(a_{41}A_{31} + a_{42}A_{23} + a_{43}A_{33})/D$$

in which A_{ij} is the co-factor of a_{ij} in D . The substitution $x_i = w_i + \alpha_i$ then leads to

$$a_{11}w_1^2 + a_{22}w_2^2 + a_{33}w_3^2 + 2a_{12}w_1w_2 + 2a_{23}w_2w_3 + 2a_{31}w_3w_1 + S/D = 0 \quad \dots (22)$$

(Continued on next page)

TABLE 2.2.5.3 (continued)

Reduction to Principal Axes

The quadratic terms in either (21) or (22) can be reduced to a sum of squares by the methods of Section 2.1.8.6 (page 13).

NOTE. When \pm signs are shown, corresponding signs must be taken throughout. Thus in entries (1) and (2) below the three λ 's must have the same sign. When the roots differ in sign λ_1 is arbitrarily taken as positive and λ_3 taken as negative. λ_2 may then have either sign. An asterisk indicates that the corresponding quantity may take any value irrespective of the signs of other entries but subject to the other conditions specified. Thus in entries (5) and (6) D may have any non-zero value. In entries (11) and (14) δ may have any value.

CASE I. $D \neq 0$.

Transform to centre and to principal axes: $\lambda_1 y_1^2 + \lambda_2 y_2^2 + \lambda_3 y_3^2 + S/D = 0$.

	λ_1	λ_2	λ_3	D	S	Standard Form	Conicoid	Special Cases
1	\pm	\pm	\pm	\pm	$-$	$X^2/A^2 + Y^2/B^2 + Z^2/C^2 = 1$	Ellipsoid	Prolate or oblate spheroid; sphere
2	\pm	\pm	\pm	\pm	$+$	$X^2/A^2 + Y^2/B^2 + Z^2/C^2 = -1$	Imaginary ellipsoid	Imaginary spheroids or sphere
3	$+$	\mp	$-$	\pm	$+$	$X^2/A^2 + Y^2/B^2 - Z^2/C^2 = 1$	Hyperboloid of one sheet (unparted)	Hyperboloid of revolution (unparted)
4	$+$	\mp	$-$	\pm	$-$	$X^2/A^2 + Y^2/B^2 - Z^2/C^2 = -1$	Hyperboloid of two sheets (parted)	Hyperboloid of revolution (parted)
5	$+$	\pm	$-$	*	0	$X^2/A^2 + Y^2/B^2 - Z^2/C^2 = 0$	Cone	Circular cone
6	\pm	\pm	\pm	*	0	$X^2/A^2 + Y^2/B^2 + Z^2/C^2 = 0$	Imaginary cone with real vertex	Three unnamed special cases

CASE II. $D=0$; $\lambda_3=0$.

Transform to principal axes: $\lambda_1 y_1^2 + \lambda_2 y_2^2 + 2\nu_1 y_1 + 2\nu_2 y_2 + 2\nu_3 y_3 + d = 0$.

Reduce linear terms by completion of squares: $\lambda_1 z_1^2 + \lambda_2 z_2^2 + 2\nu_3 y_3 + \delta = 0$.

CASE IIa. $\nu_3 \neq 0$.

Reduce to form: $\lambda_1 z_1^2 + \lambda_2 z_2^2 + 2\nu_3 z_3 = 0$ by shift of origin of y_3 to vertex of paraboloid.

	λ_1	λ_2	Standard Form	Conicoid	Special Cases
7	\pm	\pm	$X^2/A^2 + Y^2/B^2 = \pm 2Z$	Elliptic paraboloid	Paraboloid of revolution
8	$+$	$-$	$X^2/A^2 - Y^2/B^2 = \pm 2Z$	Hyperbolic paraboloid	

CASE IIb: $\nu_3 = 0$.

	λ_1	λ_2	δ	Standard Form	Conicoid	Special Cases
9	\pm	\pm	\mp	$X^2/A^2 + Y^2/B^2 = 1$	Elliptic cylinder	Circular cylinder Imaginary circular cylinder
10	\pm	\pm	\pm	$X^2/A^2 + Y^2/B^2 = -1$	Imaginary elliptic cylinder	
11	$+$	$-$	*	$X^2/A^2 - Y^2/B^2 = 1$	Hyperbolic cylinder	
12	$+$	$-$	0	$X^2/A^2 - Y^2/B^2 = 0$	Pair of real intersecting planes	
13	\pm	\pm	0	$X^2/A^2 + Y^2/B^2 = 0$	Pair of imaginary planes with real line of intersection	

(Continued on next page)

TABLE 2.2.5.3 (continued)

CASE III: $D=0$; $\lambda_2=\lambda_3=0$.Transform to principal axes: $\lambda_1 y_1^2 + 2\nu_1 y_1 + 2\nu_2 y_2 + 2\nu_3 y_3 + d = 0$.Reduce linear term in y_1 by completion of the square and the remaining terms by the substitution $z_2 = \nu_2 y_2 + \nu_3 y_3$ and obtain $\lambda_1 z_1^2 + 2\nu_2 z_2 + \delta = 0$.

	λ_1	ν_2	δ	Standard Form	Conicoid
14	$\neq 0$	$\neq 0$	*	$Y^2 = \pm 4AZ$	Parabolic cylinder
15	\pm	0	\mp	$Y^2 = A^2$	Pair of real parallel planes
16	\pm	0	0	$Y^2 = 0$	Pair of coincident planes

2.2.5.4. GENERAL PROPERTIES OF SURFACES

In general, a real straight line intersects a real surface of the n th degree in n points.

If the equation of the surface is given in the form

$$\phi(x, y, z) = 0$$

the equation of the tangent plane at the point $x_0 y_0 z_0$ (on the surface) will be

$$(x-x_0)\left(\frac{\partial\phi}{\partial x}\right)_0 + (y-y_0)\left(\frac{\partial\phi}{\partial y}\right)_0 + (z-z_0)\left(\frac{\partial\phi}{\partial z}\right)_0 = 0 \quad \dots (23)$$

For detailed discussion of the properties of surfaces, reference is made to advanced textbooks of analytical geometry.

2.2.5.5. PROPERTIES OF REGULAR SOLIDS (In collaboration with P. J. Brown and H. D. Megaw)

A convex polyhedron is said to be *regular* if its faces are regular and equal, while its vertices are all surrounded alike. There are five regular convex polyhedra, the so-called Platonic solids. These are the tetrahedron, cube, octahedron, icosahedron and pentagonal dodecahedron. While the icosahedron and pentagonal dodecahedron are not crystallographic solids, they are of importance in crystal structure problems since the neighbouring atoms of a given atom may occur in these configurations.

A polyhedron is said to be *facially regular* if every face is a regular polygon, though the faces are not all of the same kind, and if the faces are arranged in the same order round each vertex. There are thirteen such solids, and only one example—the cuboctahedron—is described here. Also there are thirteen polyhedra which are regular in respect to their vertices and in each of which the faces are equal. These are related

to the facially regular solids by the principle of *duality*, whereby vertices and faces are interchanged. The rhombic dodecahedron is the one example of a “vertex-regular” solid of special significance crystallographically. It is the dual of the cuboctahedron.

A detailed discussion of various polyhedra may be found in references [32] and [33].

For all convex polyhedra Euler's theorem states that $V + F = E + 2$, where V , F , E are respectively the number of vertices, faces and edges.

In the Tables, vertices are given in Cartesian co-ordinates. In each polyhedron the most important dimensions are given in terms of a simple choice of co-ordinates for the vertices. These dimensions are expressed (both operationally and in decimals) in terms of the units chosen for the vertices. The co-ordinates of the vertices and dimensions are also similarly specified for polyhedra of unit edge, and in cases (c) to (g) for unit distance from centre to vertex.

TABLE 2.2.5.5
Dimensions of Regular Solids

(a) Cube

$$V=8, F=6, E=12$$

$$\text{Dihedral angle} = 90^\circ$$

Vertices ..	$(\pm 1, \pm 1, \pm 1)$	$(\pm 1/2, \pm 1/2, \pm 1/2)$
Edge	2	1
Face diagonal	$2\sqrt{2}$	$\sqrt{2}$
Body diagonal	$2\sqrt{3}$	$\sqrt{3}$
Area of face ..	4	1
Volume ..	8	1

(Continued on next page)

TABLE 2.2.5.5 (continued)

(b) Tetrahedron

$V=4, F=4, E=6$

Dihedral angle = $70^\circ 32'$

Vertices	$(1, 1, 1) (1, -1, -1)$ $(-1, 1, -1) (-1, -1, 1)$		$\left(\frac{1}{2\sqrt{2}}, \frac{1}{2\sqrt{2}}, \frac{1}{2\sqrt{2}}\right) \left(\frac{1}{2\sqrt{2}}, \frac{-1}{2\sqrt{2}}, \frac{-1}{2\sqrt{2}}\right)$ $\left(\frac{-1}{2\sqrt{2}}, \frac{1}{2\sqrt{2}}, \frac{-1}{2\sqrt{2}}\right) \left(\frac{-1}{2\sqrt{2}}, \frac{-1}{2\sqrt{2}}, \frac{1}{2\sqrt{2}}\right)$	
Centre to mid edge	1	1	$1/(2\sqrt{2})$	0.35355
Centre to centre of face ..	$1/\sqrt{3}$	0.57735	$1/(2\sqrt{6})$	0.20412
Centre to vertex	$\sqrt{3}$	1.73205	$\sqrt{(3/8)}$	0.61237
Edge	$2\sqrt{2}$	2.82843	1	1
Mid edge to centre of face ..	$\sqrt{(2/3)}$	0.81650	$1/(2\sqrt{3})$	0.28868
Mid edge to vertex	$\sqrt{6}$	2.44949	$(\sqrt{3})/2$	0.86603
Mid edge to opposite mid edge	2	2	$1/\sqrt{2}$	0.70711
Height (vertex to centre of opposite face)	$4/\sqrt{3}$	2.30940	$\sqrt{(2/3)}$	0.81650
Area of face	$2\sqrt{3}$	3.46410	$(\sqrt{3})/4$	0.43301
Volume	$8/3$	2.66667	$1/(6\sqrt{2})$	0.11785

(c) Octahedron

$V=6, F=8, E=12$

Dihedral angle = $109^\circ 28'$

Vertices	$(\pm 1, 0, 0)$ $(0, \pm 1, 0)$ $(0, 0, \pm 1)$		$\left(\pm \frac{1}{\sqrt{2}}, 0, 0\right)$ $\left(0, \pm \frac{1}{\sqrt{2}}, 0\right)$ $\left(0, 0, \pm \frac{1}{\sqrt{2}}\right)$	
Edge	$\sqrt{2}$	1.41421	1	1
Centre to vertex	1	1	$1/\sqrt{2}$	0.70711
Centre to mid edge	$1/\sqrt{2}$	0.70711	$1/2$	0.50000
Centre to centre of face ..	$1/\sqrt{3}$	0.57735	$1/\sqrt{6}$	0.40825
Mid edge to near vertex ..	$\sqrt{(3/2)}$	1.22474	$(\sqrt{3})/2$	0.86603
Mid edge to distant vertex ..	$\sqrt{(5/2)}$	1.58114	$(\sqrt{5})/2$	1.11803
Area of face	$(\sqrt{3})/2$	0.86603	$(\sqrt{3})/4$	0.43301
Volume	$4/3$	1.33333	$(\sqrt{2})/3$	0.47140

(Continued on next page)

TABLE 2.2.5.5 (continued)

(d) Rhombic Dodecahedron

$V=14, F=12, E=24$

Dihedral angle = 120°

Vertices	6 Tetragonal ..	$(\pm 1, 0, 0) (0, \pm 1, 0) (0, 0, \pm 1)$		$\left(\pm \frac{2}{\sqrt{3}}, 0, 0\right) \left(0, \pm \frac{2}{\sqrt{3}}, 0\right) \left(0, 0, \pm \frac{2}{\sqrt{3}}\right)$	
	8 Trigonal ..	$(\pm 1/2, \pm 1/2, \pm 1/2)$		$\left(\pm \frac{1}{\sqrt{3}}, \pm \frac{1}{\sqrt{3}}, \pm \frac{1}{\sqrt{3}}\right)$	
Centre to tet. vertices ..	1	1	$2/\sqrt{3}$	1.15470	
Centre to trig. vertices ..	$(\sqrt{3})/2$	0.86603	1	1	
Centre to centre of faces ..	$1/\sqrt{2}$	0.70711	$\sqrt{(2/3)}$	0.81650	
Edge (trig. vert. to tet. vert.)	$(\sqrt{3})/2$	0.86603	1	1	
Centre of face to tet. vert. ..	$1/\sqrt{2}$	0.70711	$\sqrt{(2/3)}$	0.81650	
Centre of face to trig. vert. ..	1/2	0.50000	$1/\sqrt{3}$	0.57735	
Area of face	$1/\sqrt{2}$	0.70711	$(2\sqrt{2})/3$	0.94281	
Volume	2	2	$16/(3\sqrt{3})$	3.07920	

(e) Regular (pentagonal) Dodecahedron

$V=20, F=12, E=30$

Dihedral angle = $116^\circ 34'$

Vertices†	$\left(0, \pm \frac{1}{\tau}, \pm \tau\right)$		$\left(0, \pm \frac{1}{2}, \pm \frac{\tau^2}{2}\right)$		$\left(0, \pm \frac{1}{\tau\sqrt{3}}, \pm \frac{\tau}{\sqrt{3}}\right)$	
	$\left(\pm \tau, 0, \pm \frac{1}{\tau}\right)$		$\left(\pm \frac{\tau^2}{2}, 0, \pm \frac{1}{2}\right)$		$\left(\pm \frac{\tau}{\sqrt{3}}, 0, \pm \frac{1}{\tau\sqrt{3}}\right)$	
	$\left(\pm \frac{1}{\tau}, \pm \tau, 0\right)$		$\left(\pm \frac{1}{2}, \pm \frac{\tau^2}{2}, 0\right)$		$\left(\pm \frac{1}{\tau\sqrt{3}}, \pm \frac{\tau}{\sqrt{3}}, 0\right)$	
	$(\pm 1, \pm 1, \pm 1)$		$\left(\pm \frac{\tau}{2}, \pm \frac{\tau}{2}, \pm \frac{\tau}{2}\right)$		$\left(\pm \frac{1}{\sqrt{3}}, \pm \frac{1}{\sqrt{3}}, \pm \frac{1}{\sqrt{3}}\right)$	
Edge	$\frac{2}{\tau}$	1.23607	1	1	$\frac{2}{\tau\sqrt{3}}$	0.71364
Centre to vertex ..	$\sqrt{3}$	1.73205	$\frac{\tau\sqrt{3}}{2}$	1.40126	1	1
Centre to mid edge ..	τ	1.61803	$\frac{\tau^2}{2}$	1.30902	$\frac{\tau}{\sqrt{3}}$	0.93417
Centre to centre of face	$\frac{\tau^{3/2}}{5^{1/4}}$	1.37638	$\frac{\tau^{5/2}}{2(5^{1/4})}$	1.11352	$\frac{\tau^{3/2}}{5^{1/4}\sqrt{3}}$	0.79465
Area of face	$\frac{5^{3/4}}{\sqrt{\tau}}$	2.62866	$\frac{5^{3/4}\tau^{3/2}}{4}$	1.72048	$\frac{5^{3/4}}{3\sqrt{\tau}}$	0.87622
Volume	$4\tau\sqrt{5}$	14.47214	$\frac{\tau^4\sqrt{5}}{2}$	7.66312	$\frac{4\tau}{3}\sqrt{\frac{5}{3}}$	2.78516

$$\dagger \tau = \frac{1+\sqrt{5}}{2} = 1.61803; 1/\tau = \tau - 1; \tau^2 = \tau + 1; \tau\sqrt{5} = \tau + 2.$$

(Continued on next page)

2.2. TRIGONOMETRY AND GEOMETRY

TABLE 2.2.5.5 (*continued*)

(f) Icosahedron

$V=12, F=20, E=30$
Dihedral angle= $138^\circ 12'$

Vertices†	$\left(0, \pm\frac{\tau}{2}, \pm\frac{1}{2}\right)$ $\left(\pm\frac{1}{2}, 0, \pm\frac{\tau}{2}\right)$ $\left(\pm\frac{\tau}{2}, \pm\frac{1}{2}, 0\right)$		$\left(0, \pm 1, \pm\frac{1}{\tau}\right)$ $\left(\pm\frac{1}{\tau}, 0, \pm 1\right)$ $\left(\pm 1, \pm\frac{1}{\tau}, 0\right)$		$\left(0, \pm\frac{\sqrt{\tau}}{5^{1/4}}, \pm\frac{1}{5^{1/4}\sqrt{\tau}}\right)$ $\left(\pm\frac{1}{5^{1/4}\sqrt{\tau}}, 0, \pm\frac{\sqrt{\tau}}{5^{1/4}}\right)$ $\left(\pm\frac{\sqrt{\tau}}{5^{1/4}}, \pm\frac{1}{5^{1/4}\sqrt{\tau}}, 0\right)$	
Edge	1	1	$\frac{2}{\tau}$	1.23607	$\frac{2}{5^{1/4}\sqrt{\tau}}$	1.05146
Centre to vertex ..	$\frac{5^{1/4}\sqrt{\tau}}{2}$	0.95106	$\frac{5^{1/4}}{\sqrt{\tau}}$	1.17557	1	1
Centre to mid edge ..	$\frac{\tau}{2}$	0.80902	1	1	$\frac{\sqrt{\tau}}{5^{1/4}}$	0.85065
Centre to centre of face	$\frac{\tau^2}{2\sqrt{3}}$	0.75576	$\frac{\tau}{\sqrt{3}}$	0.93417	$\frac{\tau^{3/2}}{5^{1/4}\sqrt{3}}$	0.79465
Area of face	$\frac{\sqrt{3}}{4}$	0.43301	$\frac{\sqrt{3}}{\tau^2}$	0.66158	$\frac{1}{\tau}\sqrt{\frac{3}{5}}$	0.47873
Volume	$\frac{5\tau^2}{6}$	2.18169	$\frac{20}{3\tau}$	4.12023	$\frac{4(5^{1/4})\sqrt{\tau}}{3}$	2.53615

$$\dagger \tau = \frac{1+\sqrt{5}}{2} = 1.61803; \quad 1/\tau = \tau - 1; \quad \tau^2 = \tau + 1; \quad \tau\sqrt{5} = \tau + 2.$$

(g) Cuboctahedron

$V=12, F=14, E=24$
Dihedral angle= $125^\circ 16'$

Vertices	$(0, \pm 1, \pm 1)$ $(\pm 1, 0, \pm 1)$ $(\pm 1, \pm 1, 0)$		$\left(0, \pm\frac{1}{\sqrt{2}}, \pm\frac{1}{\sqrt{2}}\right)$ $\left(\pm\frac{1}{\sqrt{2}}, 0, \pm\frac{1}{\sqrt{2}}\right)$ $\left(\pm\frac{1}{\sqrt{2}}, \pm\frac{1}{\sqrt{2}}, 0\right)$	
Edge	$\sqrt{2}$	1.41421	1	1
Centre to vertex	$\sqrt{2}$	1.41421	1	1
Centre to mid edge	$\sqrt{(3/2)}$	1.22474	$(\sqrt{3})/2$	0.86603
Centre to centre of square face ..	1	1	$1/\sqrt{2}$	0.70711
Centre to centre of triangular face	$2/\sqrt{3}$	1.15470	$\sqrt{(2/3)}$	0.81650
Vertex to centre of square face ..	1	1	$1/\sqrt{2}$	0.70711
Vertex to centre of triangular face	$\sqrt{(2/3)}$	0.81650	$1/\sqrt{3}$	0.57735
Area of square face	2	2	1	1
Area of triangular face	$(\sqrt{3})/2$	0.86603	$(\sqrt{3})/4$	0.43301
Volume	$20/3$	6.66667	$5(\sqrt{2})/3$	2.35702

2.3. Differential and Integral Calculus

2.3.1. Differential Calculus

(a) Definitions and Notations

$$(1) \quad dy/dx = df(x)/dx = \lim_{h \rightarrow 0} \{f(x+h) - f(x)\}/h.$$

$$(2) \quad \partial f(x, y, z)/\partial y = \lim_{h \rightarrow 0} \{f(x, y+h, z) - f(x, y, z)\}/h, \text{ etc.}$$

$$(3) \quad d^2y/dx^2 = \frac{d}{dx} \left(\frac{dy}{dx} \right), \text{ etc.}$$

$$(4) \quad \frac{\partial^2 f}{\partial x \partial y} = \frac{\partial}{\partial x} \left(\frac{\partial f}{\partial y} \right) = \frac{\partial}{\partial y} \left(\frac{\partial f}{\partial x} \right), \text{ etc.}$$

(b) Basic Forms

$$(5) \quad d(u+v)/dx = \frac{du}{dx} + \frac{dv}{dx}.$$

$$(6) \quad d(uv)/dx = u \frac{dv}{dx} + v \frac{du}{dx}.$$

$$(7) \quad d(u/v)/dx = \left(v \frac{du}{dx} - u \frac{dv}{dx} \right) / v^2.$$

$$(8) \quad df(u)/dx = \frac{df}{du} \frac{du}{dx}.$$

$$(9) \quad d^2f(u)/dx^2 = \frac{df}{du} \frac{d^2u}{dx^2} + \frac{d^2f}{du^2} \left(\frac{du}{dx} \right)^2.$$

If $x = \phi(y)$ and $\phi'(y) = d\phi/dy$, etc.:

$$(10) \quad dy/dx = \frac{1}{\phi'(y)}; \quad d^2y/dx^2 = -\phi''(y)/[\phi'(y)]^3.$$

If $x = f(t)$ and $y = \phi(t)$:

$$(11) \quad \frac{dy}{dx} = \frac{\phi'}{f'}, \quad \frac{d^2y}{dx^2} = \frac{f'\phi'' - f''\phi'}{[f']^3}.$$

If $f(x, y) = 0$:

$$(12) \quad \frac{dy}{dx} = -\frac{\partial f/\partial x}{\partial f/\partial y};$$

$$\frac{d^2y}{dx^2} = -\frac{\frac{\partial^2 f}{\partial x^2} \left(\frac{\partial f}{\partial y} \right)^2 - 2 \frac{\partial^2 f}{\partial x \partial y} \frac{\partial f}{\partial x} \frac{\partial f}{\partial y} + \frac{\partial^2 f}{\partial y^2} \left(\frac{\partial f}{\partial x} \right)^2}{\left(\frac{\partial f}{\partial y} \right)^3}.$$

If $y = f(u, v)$ and $u = \phi(x)$ and $v = \psi(x)$:

$$(13) \quad \frac{dy}{dx} = \frac{\partial y}{\partial u} \frac{du}{dx} + \frac{\partial y}{\partial v} \frac{dv}{dx}$$

$$\frac{d^2y}{dx^2} = \frac{\partial^2 y}{\partial u^2} \left(\frac{du}{dx} \right)^2 + 2 \frac{\partial^2 y}{\partial u \partial v} \frac{du}{dx} \frac{dv}{dx} + \frac{\partial^2 y}{\partial v^2} \left(\frac{dv}{dx} \right)^2$$

$$+ \frac{\partial y}{\partial u} \frac{d^2u}{dx^2} + \frac{\partial y}{\partial v} \frac{d^2v}{dx^2}.$$

If $V = \phi(u, v)$ and $u = f_1(x, y)$ and $v = f_2(x, y)$:

$$(14) \quad \frac{\partial V}{\partial x} = \frac{\partial V}{\partial u} \frac{\partial u}{\partial x} + \frac{\partial V}{\partial v} \frac{\partial v}{\partial x}$$

$$\frac{\partial^2 V}{\partial x^2} = \frac{\partial^2 V}{\partial u^2} \left(\frac{\partial u}{\partial x} \right)^2 + \frac{\partial^2 V}{\partial v^2} \left(\frac{\partial v}{\partial x} \right)^2 + 2 \frac{\partial^2 V}{\partial u \partial v} \frac{\partial u}{\partial x} \frac{\partial v}{\partial x}$$

$$+ \frac{\partial V}{\partial u} \frac{\partial^2 u}{\partial x^2} + \frac{\partial V}{\partial v} \frac{\partial^2 v}{\partial x^2}$$

$$= \left(\frac{\partial u}{\partial x} \frac{\partial}{\partial u} + \frac{\partial v}{\partial x} \frac{\partial}{\partial v} \right) \left(\frac{\partial V}{\partial u} \frac{\partial u}{\partial x} + \frac{\partial V}{\partial v} \frac{\partial v}{\partial x} \right)$$

$$\frac{\partial^2 V}{\partial x \partial y} = \frac{\partial^2 V}{\partial u^2} \frac{\partial u}{\partial x} \frac{\partial u}{\partial y} + \frac{\partial^2 V}{\partial u \partial v} \left(\frac{\partial v}{\partial x} \frac{\partial u}{\partial y} + \frac{\partial u}{\partial x} \frac{\partial v}{\partial y} \right)$$

$$+ \frac{\partial^2 V}{\partial v^2} \frac{\partial v}{\partial x} \frac{\partial v}{\partial y} + \frac{\partial V}{\partial u} \frac{\partial^2 u}{\partial x \partial y} + \frac{\partial V}{\partial v} \frac{\partial^2 v}{\partial x \partial y}$$

$$= \left(\frac{\partial u}{\partial x} \frac{\partial}{\partial u} + \frac{\partial v}{\partial x} \frac{\partial}{\partial v} \right) \left(\frac{\partial V}{\partial u} \frac{\partial u}{\partial y} + \frac{\partial V}{\partial v} \frac{\partial v}{\partial y} \right)$$

(c) Derivatives of Simple Functions

$$(15) \quad \frac{dx^n}{dx} = nx^{n-1}.$$

$$(16) \quad \frac{de^{ax}}{dx} = ae^{ax}.$$

$$(17) \quad \frac{da^u}{dx} = a^u \frac{du}{dx} \ln a.$$

$$(18) \quad \frac{d \sin x}{dx} = \cos x.$$

$$(19) \quad \frac{d \cos x}{dx} = -\sin x.$$

$$(20) \quad \frac{d \tan x}{dx} = \sec^2 x.$$

(d) Taylor's Series

$$(21) \quad f(x_0 + h) = f(x_0) + h \left(\frac{df}{dx} \right)_0 + \frac{h^2}{2!} \left(\frac{d^2f}{dx^2} \right)_0 + \dots$$

$$+ \frac{h^n}{n!} \left(\frac{d^n f}{dx^n} \right)_0$$

If $f(x)$ and its derivatives are finite and continuous within the range $x_0 - h < x < x_0 + h$, then the series (21) differs from $f(x)$ by an amount no greater than R_{n+1} where

$$R_{n+1} = \frac{h^{n+1}}{(n+1)!} M_{n+1}$$

where M_{n+1} is the upper bound of f^{n+1} within the range.

$$(22) \quad f(x_0 + u, y_0 + v) = f(x_0, y_0) + \left(u \frac{\partial f}{\partial x} + v \frac{\partial f}{\partial y} \right)_0$$

$$+ \frac{1}{2!} \left(u^2 \frac{\partial^2 f}{\partial x^2} + 2uv \frac{\partial^2 f}{\partial x \partial y} + v^2 \frac{\partial^2 f}{\partial y^2} \right)_0 + \dots$$

$$+ \frac{1}{n!} \left(u \frac{\partial}{\partial x} + v \frac{\partial}{\partial y} \right)^n f(x_0, y_0)$$

This series represents $f(x, y)$ within the range to an accuracy R_{n+1} where R_{n+1} is less than or equal to the upper bound in the range of the first omitted term.

(e) *Differentiation of an Integral*

$$(23) \quad y = \int_a^x f(x) dx; \quad \frac{dy}{dx} = f(x).$$

$$(24) \quad y = \int_a^b f(x, u) dx; \quad \frac{dy}{du} = \int_a^b \frac{\partial f}{\partial u} dx.$$

$$(25) \quad y = \int_{x_0(\alpha)}^{x_1(\alpha)} v(x, \alpha) dx; \quad \frac{dy}{d\alpha} = \int_{x_0}^{x_1} \frac{\partial v}{\partial \alpha} dx + v(x_1, \alpha) \frac{dx_1}{d\alpha} - v(x_0, \alpha) \frac{dx_0}{d\alpha}.$$

For further tables of derivatives see [2], [6]–[9].

2.3.2. Integral Calculus

2.3.2.1. INDEFINITE INTEGRALS

It is impossible within the scope of these tables to give a list of indefinite integrals which is extensive enough to be of value. For such lists see the bibliography.

2.3.2.2. DEFINITE INTEGRALS

The following definite integrals are of sufficient frequency of occurrence in crystallographic calculations to merit listing here.

$$(1) \quad \int_0^{\frac{\pi}{2}} \sin^n x \, dx = \int_0^{\frac{\pi}{2}} \cos^n x \, dx$$

$$= \frac{1.3.5 \dots (n-1)}{2.4.6 \dots n} \frac{\pi}{2} \quad (n \text{ even})$$

$$= \frac{2.4.6 \dots (n-1)}{1.3.5.7 \dots n} \quad (n \text{ odd})$$

$$(2) \quad \int_0^{2\pi} \sin^n x \, dx = \int_0^{2\pi} \cos^n x \, dx = 0 \quad (n \text{ odd})$$

$$= \frac{1.3.5 \dots (n-1)}{2.4.6 \dots n} \cdot 2\pi \quad (n \text{ even})$$

$$(3) \quad \int_0^{2\pi} \sin mx \sin nx \, dx = \int_0^{2\pi} \cos mx \cos nx \, dx$$

$$= 0 \quad (m \neq n), \quad = \pi \quad (m = n)$$

$$\int_0^{2\pi} \sin mx \cos nx \, dx = 0 \quad (\text{all } m, n)$$

$$(4) \quad \int_0^{2\pi} e^{imx} dx = 0 \quad (m \neq 0), \quad = 2\pi \quad (m = 0).$$

$$(5.1) \quad \int_0^{\infty} \frac{\sin x}{x} dx = \frac{\pi}{2}.$$

$$(5.2) \quad \int_0^{\infty} \left[\frac{\sin x}{x} \right]^2 dx = \frac{\pi}{2}.$$

$$(5.3) \quad \int_0^{\infty} \left[\frac{\sin x}{x} \right]^3 dx = \frac{3\pi}{8}.$$

$$(5.4) \quad \int_0^{\infty} \left[\frac{\sin x}{x} \right]^4 dx = \frac{\pi}{3} \dagger$$

$$(6) \quad \int_0^{\infty} x^n e^{-ax} dx = n! / a^{n+1}.$$

$$(7.1) \quad \int_0^{\infty} x^{2n} e^{-ax^2} dx = \frac{(2n)!}{2^{2n+1} a^n n!} \sqrt{\frac{\pi}{a}}.$$

$$(7.2) \quad \int_0^{\infty} x^{2n+1} e^{-ax^2} dx = n! / 2a^{n+1}.$$

$$(7.3) \quad \int_0^{\infty} e^{-ax^2} dx = \frac{1}{2} \sqrt{\frac{\pi}{a}}.$$

$$(7.4) \quad \int_0^{\infty} x^2 e^{-ax^2} dx = \frac{1}{4a} \sqrt{\frac{\pi}{a}}.$$

If the Fourier Transform of any function is known, its definite integral over the doubly infinite range is also known from the obvious formulae

$$f(0) = \int_{-\infty}^{\infty} F(u) du \quad \text{and} \quad F(0) = \int_{-\infty}^{\infty} f(x) dx$$

For references to tables of Fourier Transforms see [62]–[66].

For references in connection with Section 2.3.2 generally, see any textbook of the integral calculus and also [2], [6]–[9]. The basic tabulation of definite integrals is [34]. For methods for the evaluation of definite integrals by contour integration see any text on the theory of functions of a complex variable, e.g. [12] and [13].

† For general formula see [13], Chapter VI, Misc. Ex. 13.

2.4. Vector and Tensor Analysis

2.4.1. Definitions

A *scalar* is a quantity which is defined by its magnitude (a single number) in a space of n dimensions. A sign may also be allotted to a scalar.

A *vector* is a quantity which is defined by its direction and magnitude. In n dimensions, n numbers are required for its definition.

A *tensor* of order p requires n^p numbers for its definition in n dimensions. A vector is a first order tensor, and a scalar a zero order tensor. A second order tensor will in general express the relationship between two vectors, and in general a tensor of order p will express relationship between two tensors of lower order p_1 and p_2 such that $p=p_1+p_2$. Detailed definitions of some of the many types of tensors are given in Section 2.4.4 (page 54).

Many techniques have been suggested for handling the mathematics of vectors and of tensors, and there has been considerable controversy as to their relative merits. Some vector properties can be stated without reference to any co-ordinate system (2.4.2). However, in almost all calculations involving vectors reference must ultimately be made to a co-ordinate system. Of the many techniques developed for handling vectors and second order tensors the two most fruitful have been the dyadics of Willard Gibbs and the tensor analysis of Ricci and Levi-Civita. The calculations which result from such methods can be included in matrix analysis (Section 2.1.8, page 11).

For a historical summary see [39].

2.4.2. Absolute Vector Analysis

Some results of vector analysis can be expressed without reference to any co-ordinate system.

(a) The *scalar product* of two vectors a and b , of magnitudes a and b respectively, is the scalar quantity

$$a.b \equiv (ab) = ab \cos \theta \quad \dots (1)$$

if the forward directions of the two vectors make an angle θ with one another.

The "dot" notation and the "parenthesis" notation are used interchangeably in these tables and are both in current use in the literature. The scalar product is commutative, i.e.

$$(ab) = (ba) \quad \dots (2)$$

(b) The *vector product* of two vectors a and b is a vector c at right angles to both a and b , in the sense that a, b, c taken in that order form a *right-handed system*, i.e. a right-handed rotation through an angle less than 180° in the direction c takes a into b . The magnitude c of the vector c is given by

$$c = ab \sin \theta \quad \dots (3)$$

where the angle θ is measured as a right-handed

rotation from a to b about c . There are again two standard notations for the vector product

$$a \times b \equiv [ab] = c \quad \dots (4)$$

Occasionally the redundant notation $[a \times b]$ is convenient if a and b are themselves composite, but it should be avoided if possible. The vector product does not *commute*, i.e.

$$a \times b = -b \times a = c \quad \dots (5)$$

(c) The magnitude $a = |a|$ of a vector a is defined by

$$a^2 = |a|^2 = a.a \quad \dots (6)$$

(d) The *multiplication of a vector a by a scalar s* results in a vector of magnitude sa in the same direction as a , although the sense of sa will be opposite to that of a if s is negative.

(e) The simplest type of vector is a *displacement*, but a vector may represent any directed quantity such as a velocity, acceleration, force, field, etc. However, any vector may be represented by a displacement.

(f) The *addition or subtraction of two vectors* follows the parallelogram law for displacements. The magnitude of the sum of two vectors $a+b=c$ is given by

$$c^2 = |a+b|^2 = a^2 + b^2 + 2ab \cos \theta \quad \dots (7)$$

(g) The *scalar triple product* of three vectors abc is

$$a.[bc] = \pm v \quad \dots (8a)$$

where

$$v = abc(1 - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma + 2 \cos \alpha \cos \beta \cos \gamma)^{\frac{1}{2}} \quad \dots (8b)$$

and α, β, γ are respectively the angles between b and c , c and a , and a and b . The sign allotted to v is $+$ if a, b, c taken in order form a right-handed system and $-$ if they form a left-handed system. The volume of the parallelepiped bounded by the three vectors a, b, c is $|v|$. We thus have

$$a.[bc] = b.[ca] = c.[ab] = -a.[cb] = -c.[ba] = -b.[ac] \quad \dots (8c)$$

The simplified notation (abc) is often used for this product.

(h) The *vector triple product* is non-associative, and there are two important forms:

$$a \times [bc] = (ca)b - (ab)c \quad \dots (9a)$$

$$[ab] \times c = (ca)b - (bc)a \quad \dots (9b)$$

(i) The *scalar four-fold product* is expandable as

$$[ab].[cd] = (ac)(bd) - (ad)(bc) \quad \dots (10)$$

(j) The *vector four-fold product* has two expansions:

$$[ab] \times [cd] = (abd)c - (abc)d \\ = (cda)b - (cdb)a \quad \dots (11)$$

(k) The solution of *vector equations* presents special features which are indicated by the following examples:

$$\text{The equation } (ab)=0 \quad \dots(12)$$

implies that *either* \mathbf{a} or \mathbf{b} or both are zero vectors, or that \mathbf{a} and \mathbf{b} are *orthogonal* ($\theta=\pi/2$).

$$\text{The equation } [ab]=0 \quad \dots(13)$$

implies that *either* \mathbf{a} or \mathbf{b} or both are zero vectors, or that \mathbf{a} and \mathbf{b} are *collinear* ($\theta=0$), and hence that

$$\mathbf{a}=(ab)\mathbf{b}/(bb) \quad \dots(13a)$$

$$\text{The equation } (abc)=0 \quad \dots(14)$$

implies *either* that one or more of the vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ is zero or that all three lie in the same plane. In the latter case the three vectors are *linearly dependent*, and we have a relation of the type

$$\alpha\mathbf{a}+\beta\mathbf{b}+\gamma\mathbf{c}=0 \quad \dots(14a)$$

However, the constants α, β, γ are not determined by (14) and must follow from the known properties of the vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}$ as in (13a).

2.4.3. Base Systems and their Reciprocal Systems

Although the many results of 2.4.2 are of great theoretical interest and importance, almost all of them require use of the methods of analytical vector analysis in their proofs and in their applications. Such methods make use of the fact that in three dimensions any vector can be expressed as a sum of three non-zero non-coplanar vectors. Three such vectors are chosen as *base*, and all other vectors under discussion are expressed in terms of this base.

2.4.3.1. SUMMATION CONVENTION

In the following sections we shall make use of the convention that any repeated index implies summation over that index for all dimensions, i.e.

$$x_i y_i = \sum_{i=1}^3 x_i y_i = x_1 y_1 + x_2 y_2 + x_3 y_3$$

If repeated indices occur in which summation is not implied, this fact will be specially noted. In the sections on tensor analysis (2.4.4) a further specialization of this convention will be made.

2.4.3.2. GENERAL BASE SYSTEMS

Consider the base system \mathbf{a}_i consisting of the three non-coplanar vectors $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$. It is then possible to define a set of *reciprocal vectors* \mathbf{a}_j^* such that

$$(\mathbf{a}_i \mathbf{a}_j^*) = \delta_{ij} \quad \dots(15)$$

where δ_{ij} is the Kronecker delta. The equations (15) have the solution

$$\mathbf{a}_i^* = [\mathbf{a}_j \mathbf{a}_k] / (\mathbf{a}_1 \mathbf{a}_2 \mathbf{a}_3) \quad \dots(16a)$$

and its inverse

$$\mathbf{a}_i = [\mathbf{a}_j^* \mathbf{a}_k^*] / (\mathbf{a}_1^* \mathbf{a}_2^* \mathbf{a}_3^*) \quad \dots(16b)$$

Any vector \mathbf{x} can then be written in the form

$$\mathbf{x} = x_i \mathbf{a}_i \quad \dots(17)$$

$$\text{where } x_i = (\mathbf{x} \mathbf{a}_i^*) \quad \dots(17a)$$

and a second vector \mathbf{y} written in the same form will be

$$\mathbf{y} = y_i \mathbf{a}_i \quad \dots(17b)$$

Their scalar product will then be

$$(\mathbf{x} \mathbf{y}) = x_i y_j g_{ij} \quad \dots(18)$$

$$\text{where } (\mathbf{a}_i \mathbf{a}_j) = g_{ij} \quad \dots(18a)$$

If the second vector \mathbf{h} is expressed in the form

$$\mathbf{h} = h_i \mathbf{a}_i^* \quad \dots(19)$$

$$\text{where } h_i = (\mathbf{h} \mathbf{a}_i) \quad \dots(19a)$$

$$\text{then } (\mathbf{h} \mathbf{x}) = h_i x_i \quad \dots(20)$$

2.4.3.3. CARTESIAN BASE SYSTEMS

If the three base vectors form a right-handed system and are chosen with unit magnitude and orthogonal to one another, such a system \mathbf{e}_i is referred to as a *Cartesian* or *orthonormal* base system. It has the properties

$$(\mathbf{e}_i \mathbf{e}_j) = \delta_{ij} \quad \dots(21)$$

and it is its own reciprocal base system.

Any vector \mathbf{x} is expandable in the form

$$\mathbf{x} = x_i \mathbf{e}_i \quad \dots(22)$$

$$\text{with } x_i = (\mathbf{x} \mathbf{e}_i) \quad \dots(22a)$$

and the scalar product of any two vectors is

$$(\mathbf{x} \mathbf{y}) = x_i y_i \quad \dots(23)$$

For the vector product of two vectors we use the result

$$[\mathbf{e}_i \mathbf{e}_j] = \mathbf{e}_k = -[\mathbf{e}_j \mathbf{e}_i] \quad \dots(24)$$

and we have

$$[\mathbf{x} \mathbf{y}] = (x_2 y_3 - x_3 y_2) \mathbf{e}_1 + (x_3 y_1 - x_1 y_3) \mathbf{e}_2 + (x_1 y_2 - x_2 y_1) \mathbf{e}_3 \quad \dots(25)$$

2.4.3.4. CYLINDRICAL AND POLAR CO-ORDINATES

Cylindrical and polar co-ordinates are usually defined in terms of a Cartesian base system.

The *cylindrical* co-ordinates s, ϕ, z of the point P are defined by the relations

$$\left. \begin{aligned} x_1 &= s \cos \phi \\ x_2 &= s \sin \phi \\ x_3 &= z \end{aligned} \right\} \quad \dots(26)$$

and the vector \mathbf{r} may be written

$$\mathbf{r} = s \cos \phi \mathbf{e}_1 + s \sin \phi \mathbf{e}_2 + z \mathbf{e}_3 \quad \dots(27)$$

The scalar product of this vector with a second vector \mathbf{R} whose co-ordinates are S, Φ, Z will clearly be

$$\mathbf{r} \cdot \mathbf{R} = sS \cos(\Phi - \phi) + zZ \quad \dots(28)$$

and the lengths of these vectors will be obtained from $r^2 = s^2 + z^2$ and $R^2 = S^2 + Z^2$ respectively. The distance

between the two end points of \mathbf{r} and \mathbf{R} is obtained from

$$(\mathbf{r}-\mathbf{R})^2=s^2+S^2-2sS\cos(\Phi-\phi)+(z-Z)^2 \quad \dots(29)$$

while the volume element in these co-ordinates is

$$dV=s\,ds\,d\phi\,dz \quad \dots(30)$$

The usual ranges for these variables are $0 \leq s < \infty$; $0 \leq \phi < 2\pi$; $-\infty < z < \infty$.

The *polar co-ordinates* r, θ, ϕ of the point P are defined by the relations

$$\begin{aligned} x_1 &= r \sin \theta \cos \phi \\ x_2 &= r \sin \theta \sin \phi \\ x_3 &= r \cos \theta \end{aligned}$$

and the vector \mathbf{r} may be written

$$\mathbf{r}=r \sin \theta \cos \phi \mathbf{e}_1+r \sin \theta \sin \phi \mathbf{e}_2+r \cos \theta \mathbf{e}_3 \quad \dots(31)$$

The scalar product of this vector with a second vector \mathbf{R} whose polar co-ordinates are R, Θ, Φ will be

$$\mathbf{r}\mathbf{R}=rR[\cos \theta \cos \Theta+\sin \theta \sin \Theta \cos (\Phi-\phi)] \quad \dots(32)$$

The distance between the end points of \mathbf{r} and \mathbf{R} is obtained from

$$(\mathbf{r}-\mathbf{R})^2=r^2+R^2-2rR[\cos \theta \cos \Theta+\sin \theta \sin \Theta \cos (\Phi-\phi)] \quad \dots(33)$$

while the volume element is

$$dV=r^2 \sin \theta \,dr\,d\theta\,d\phi \quad \dots(34)$$

The usual ranges for these variables are $0 \leq r < \infty$; $0 \leq \theta < \pi$; $0 \leq \phi < 2\pi$.

2.4.3.5. THE PHYSICAL DIMENSIONS ASSOCIATED WITH BASE SYSTEMS

In setting up a Cartesian base system \mathbf{e}_i it is usual to choose the base vectors in a given set of orthogonal directions and to allot to each a *unit numerical magnitude*. In such a system the components of a vector have the same physical dimensions as the vector itself. Thus the components of a vector displacement will also be displacements and the components of a force will also have the dimensions of a force.

In setting up a general system \mathbf{a}_i in crystallography it is customary to choose the vectors \mathbf{a}_i as possessing the dimensions of length (\AA or kX). If a vector \mathbf{x} is a displacement, its components x_i as given by (17a) will be pure numbers. Similarly if the vector \mathbf{h} of (19) has dimensions of a reciprocal length, its components given by (19a) will again be pure numbers.

2.4.4. Tensor Analysis

The basic notion of tensor analysis is that *any physical or geometrical quantity must have expression in a form which remains invariant under a change of*

co-ordinate system. Thus a given vector \mathbf{x} is expressed in terms of the base system \mathbf{a}_i in the form

$$\mathbf{x}=x^i\mathbf{a}_i \quad \dots(1a)$$

while the *same vector* \mathbf{x} is expressed in terms of the system \mathbf{b}_i in the form

$$\mathbf{x}=y^i\mathbf{b}_i \quad \dots(1b)$$

The co-ordinates x^i, y^i in the two systems must be so related to the base vectors $\mathbf{a}_i, \mathbf{b}_i$ as to make the two expressions (1a) and (1b) equivalent expressions for the same vector.

In expression (1) we have used subscripts for the base vectors to indicate that they transform *in the same way as base vectors*. We shall use subscripts for all quantities which transform in this manner. These we call *covariant* quantities. The superscripts attached to the components x^i, y^i indicate that these quantities transform as do the reciprocal base vectors. Such quantities are said to be *contravariant*.

Summation will always be implied for pairs of repeated indices, and these will now always occur with one member of a pair in the covariant and the other in the contravariant position. Such indices are called *dummy indices*. It is possible to change the letters used for dummy indices at will.

Let us write

$$\mathbf{b}_i=\alpha_i^k\mathbf{a}_k \quad \dots(2a)$$

for the transformation from the base vector system \mathbf{a}_i to the base vector system \mathbf{b}_i . The inverse transformation from the system \mathbf{b}_i to the system \mathbf{a}_i will then be

$$\mathbf{a}_k=\beta_k^i\mathbf{b}_i \quad \dots(2b)$$

where the matrix β_k^i is the inverse matrix to α_i^k and is related to it by the equations (cf. 2.1.8.4)

$$\alpha_i^k\beta_k^j=\delta_i^j \quad (=0, i \neq j; =1, i=j) \quad \dots(3a)$$

and

$$\beta_i^k\alpha_k^j=\delta_i^j \quad \dots(3b)$$

To make our notation clear it is worth while to write out the matrix expressions for (3a) and (3b) in full, i.e.:

$$\begin{bmatrix} \alpha_1^1 & \alpha_1^2 & \alpha_1^3 \\ \alpha_2^1 & \alpha_2^2 & \alpha_2^3 \\ \alpha_3^1 & \alpha_3^2 & \alpha_3^3 \end{bmatrix} \begin{bmatrix} \beta_1^1 & \beta_1^2 & \beta_1^3 \\ \beta_2^1 & \beta_2^2 & \beta_2^3 \\ \beta_3^1 & \beta_3^2 & \beta_3^3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \dots(3a')$$

and

$$\begin{bmatrix} \beta_1^1 & \beta_1^2 & \beta_1^3 \\ \beta_2^1 & \beta_2^2 & \beta_2^3 \\ \beta_3^1 & \beta_3^2 & \beta_3^3 \end{bmatrix} \begin{bmatrix} \alpha_1^1 & \alpha_1^2 & \alpha_1^3 \\ \alpha_2^1 & \alpha_2^2 & \alpha_2^3 \\ \alpha_3^1 & \alpha_3^2 & \alpha_3^3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \dots(3b')$$

Thus in (3a) the subscript i is the *first* index of $[\alpha_i^k]$ and corresponds to the matrix *row* in (3a'). The superscript k is the *second* index, and this fact is indicated by the space which is left over the subscript i . The superscript k thus corresponds to the matrix *column* in the matrix $[\alpha_i^k]$. The order of the terms is chosen to correspond to the summation implied in matrix multiplication (cf. 2.1.8.2), which requires that the column index of the pre-factor corresponds to the row index of the post-factor. This ordering is not required

by the tensor notation but is used here to emphasize wherever possible the relationship of the tensor notation to the matrix notation.

We now write down (without proof) the corresponding transformations for the reciprocal triples, i.e.

$$\mathbf{b}^i = \mathbf{a}^k \beta_k^i \quad \dots (4a)$$

and its inverse

$$\mathbf{a}^k = \mathbf{b}^i \alpha_i^k \quad \dots (4b)$$

The reader can easily verify that if the triple \mathbf{a}^k is reciprocal to \mathbf{a}_k then (4a) and (4b) imply that \mathbf{b}^i and \mathbf{b}_i must also be reciprocal to one another. Note that in (2a) and (2b) the *covariant* base vectors are represented as *column* symbols in the matrix notation, since they appear as a post-multiplier, while in (4a) and (4b) the *contravariant* or reciprocal base vectors appear as *row* symbols, since they appear as a pre-multiplier.

Referring now to (1), it is clear that the *contravariant* designation for the components of \mathbf{x} was justified, since if we write

$$y^i = x^k \beta_k^i \quad \dots (5a)$$

and the inverse

$$x^k = y^i \alpha_i^k \quad \dots (5b)$$

we can verify that (1a) and (1b) are truly expressions for the same vector, i.e.

$$\mathbf{x} = x^i \mathbf{a}_i = y^k \alpha_k^i \beta_i^j \mathbf{b}_j = y^k \delta_k^j \mathbf{b}_j = y^j \mathbf{b}_j$$

We therefore call the quantities x^i and y^i the *contravariant components* of the vector \mathbf{x} in terms of the base systems \mathbf{a}_i and \mathbf{b}_i respectively. We can, however, express the same vector \mathbf{x} in terms of the reciprocal base systems \mathbf{a}^i and \mathbf{b}^i and obtain

$$\mathbf{x} = x_i \mathbf{a}^i \quad \dots (6a)$$

and also

$$\mathbf{x} = y_i \mathbf{b}^i \quad \dots (6b)$$

Here x_i and y_i are the *covariant components* of the vector \mathbf{x} . They transform according to the expressions†

$$y_i = \alpha_i^k x_k \quad \dots (7a)$$

and the inverse

$$x_k = \beta_k^i y_i \quad \dots (7b)$$

We notice that the tensor notation and its relation to the matrix notation gives a simple presentation to the transformation rules of Vol. I, 2.5. For covariant quantities the matrix which gives the new variables in terms of the old (2a) is $[\alpha_i^k]$ and the vector is a post-factor. The inverse transformation uses the inverse matrix $[\beta_k^i]$ and the vector is again a post-factor. For contravariant quantities the role of the two matrices is interchanged and the vector becomes a pre-factor.

Using the notion of transformation given above it is possible to define a set of more general quantities according to the way in which their components transform. A quantity A is defined as a second order tensor if it has n^2 components of a given variance in an n dimensional space and if its components transform as indicated below. The tensor may be represented by its *doubly covariant components* A_{ij} in the \mathbf{a}_i system and the corresponding B_{ij} in the \mathbf{b}_i system. By definition

such components must transform according to the rules

$$B_{ij} = \alpha_i^m \alpha_j^n A_{mn} \quad \dots (8a)$$

and the inverse

$$A_{mn} = \beta_m^i \beta_n^j B_{ij} \quad \dots (8b)$$

if A is to be a second order tensor. The same quantity A may be expressed in terms of its *doubly contravariant components* A^{ij} and B^{ij} in the two systems. In this case the transformations will be

$$B^{ij} = A^{mn} \beta_m^i \beta_n^j \quad \dots (9a)$$

and its inverse

$$A^{mn} = B^{ij} \alpha_i^m \alpha_j^n \quad \dots (9b)$$

We can also consider the *mixed components* A^i_j and B^i_j of the same tensor A . These will transform according to the rules

$$B^i_j = \alpha_j^n A^m_n \beta_m^i \quad \dots (10a)$$

and the inverse

$$A^m_n = \beta_n^j B^i_j \alpha_i^m \quad \dots (10b)$$

There is also a second set of mixed components A_i^j and B_i^j with covariance in the first indices and contravariance in the second. The reader can write down transformation equations for these components by analogy with (8), (9) and (10).

Note that in writing expressions (8), (9) and (10) we have not attempted to maintain the order of transformations in relation to matrix multiplication. This cannot be done without using transposed α and β matrices. Throughout the later parts of this Section we use the matrix order whenever it can be written without transposed matrices. In any case the summations implied by the dummy indices must be carried out.

The definition of higher order tensors follows directly. Thus a fourth order tensor has mixed components of the type A^{hi}_{jk} and B^{hi}_{jk} in the two systems, and these components transform according to the rule

$$B^{hi}_{jk} = \beta_p^h \beta_q^i \alpha_j^r \alpha_k^s A^{pq}_{rs} \quad \dots (11)$$

In a tensor of order r there are 2^r ways in which the components can be written as covariant or contravariant. In n dimensions a tensor of order r has n^r components of each variant configuration. Thus a vector can be taken as a first order tensor, and a scalar or invariant is a zero order tensor.

† In physical literature, particularly on relativity theory, it is customary to refer to a vector which is conveniently (for physical reasons) expressed in terms of its contravariant components as "a contravariant vector." This is very misleading, since any vector can be expressed in terms of its contravariant components or its covariant components with equal validity. In crystallography, co-ordinates of atoms are expressed in contravariant components, since these numbers repeat periodically with period unity. This is not true for the covariant components of co-ordinate vectors. Similarly zone indices are also expressed in terms of their contravariant components, since these components obey the law of rational indices, while the covariant components do not. On the other hand, the indices of planes are rational in their covariant components. There is, however, no reason other than numerical simplicity for the preference of one set of components over the other.

There is no *a priori* reason why tensors should exist other than as mathematical entities. It is necessary in any physical application of tensor analysis to demonstrate that the physical nature of the set of quantities under discussion is such that they do transform as the components of a tensor.

It is important to remember that the quantities α_i^j and β_i^j are *not* the components of a second order tensor. They express the transformation of tensors from one axial system to another.

A tensor is said to be *symmetric* (cf. 2.1.8.1) with respect to a pair of indices if the interchange of these two indices leaves the tensor unchanged, i.e. if

$$A_{ij} = A_{ji} \quad \dots (12)$$

A tensor is said to be *skew symmetric* (cf. 2.1.8.1) with respect to a pair of indices if the interchange of these indices changes the sign of the tensor, i.e. if

$$A_{ij} = -A_{ji} \quad \dots (13a)$$

For a skew symmetric tensor

$$A_{ii} = 0 \text{ (no summation)} \quad \dots (13b)$$

The most important second order tensor is the *metric tensor* g , whose components are defined by the relations

$$\begin{aligned} g_{ij} &= (\mathbf{a}_i \mathbf{a}_j) & |g| &= |g_{ij}| = |g^{ij}|^{-1} = g \\ g^{ij} &= (\mathbf{a}^i \mathbf{a}^j) & g_i^j &= g^j_i = (\mathbf{a}^i \mathbf{a}_j) = \delta^j_i \end{aligned} \quad \dots (14)$$

It is easy to verify that this tensor is symmetric and possesses the appropriate transformation properties. In terms of this tensor the length of any vector has the three expressions

$$|\mathbf{x}|^2 = g_{ij} x^i x^j = g^{ij} x_i x_j = x^i x_i \quad \dots (15)$$

The cosine of the angle θ between the two vectors \mathbf{x} and \mathbf{X} is given by

$$\begin{aligned} \cos \theta &= g_{ij} x^i X^j / |\mathbf{x}| |\mathbf{X}| = g^{ij} x_i X_j / |\mathbf{x}| |\mathbf{X}| \\ &= x^i X_i / |\mathbf{x}| |\mathbf{X}| \quad \text{etc.} \end{aligned} \quad \dots (16)$$

It is often of value to be able to define a unit vector λ in the direction of a vector \mathbf{x} . Clearly

$$\lambda_r = x_r / |\mathbf{x}| \quad \dots (17)$$

will be covariant, and its length

$$|\lambda|^2 = g^{mn} \lambda_m \lambda_n = g_{mn} \lambda^m \lambda^n = \lambda^m \lambda_m = 1 \quad \dots (18)$$

Similarly the angle between two such unit vectors λ and μ will be

$$\cos \theta = g^{mn} \lambda_m \mu_n = g_{mn} \lambda^m \mu^n = \lambda^m \mu_m \quad \dots (19)$$

The metric tensor also provides the transformation expressing the base vectors in terms of the reciprocal vectors and vice versa, i.e.

$$\mathbf{a}_i = g_{ij} \mathbf{a}^j \quad \text{and} \quad \mathbf{a}^i = g^{ij} \mathbf{a}_j \quad \dots (20)$$

and similarly the two sets of components satisfy the relations

$$x_i = g_{ij} x^j \quad \text{and} \quad x^i = g^{ij} x_j \quad \dots (21)$$

There are similar relations between the different types of components of higher order tensors, e.g.

$$A_{ij} = g_{ik} A^k_j = g_{jk} A_i^k = g_{im} g_{jn} A^{mn} \quad \dots (22)$$

and in particular

$$g_{ij} g^{jk} = \delta_i^k \quad \dots (23)$$

which establishes the matrix $[g^{ij}]$ as the inverse matrix of $[g_{ij}]$ (cf. 2.1.8.4, page 12). Note also that if A_{ij} is symmetric $A_i^k = A^i_k$.

Any second order tensor X_{mn} , say, can be expressed as the sum of a symmetric tensor S_{mn} and a skew symmetric tensor A_{mn} given by

$$\begin{aligned} S_{mn} &= \frac{1}{2}(X_{mn} + X_{nm}) \\ A_{mn} &= \frac{1}{2}(X_{mn} - X_{nm}) \end{aligned} \quad \dots (24)$$

Any second order symmetric tensor in n dimensions has $\frac{1}{2}n(n+1)$ independent components (for $n=3$, six components), while a skew symmetric tensor has $\frac{1}{2}n(n-1)$ independent components (for $n=3$, three components).

Another second order tensor of importance is the general product† of two vectors \mathbf{X} and \mathbf{Y} . It is easy to prove that

$$Z^{ij} = X^i Y^j \quad \dots (25)$$

transforms as a contravariant second order tensor. The scalar product $(\mathbf{X}\mathbf{Y})$ is then

$$(\mathbf{X}\mathbf{Y}) = g_{mn} X^m Y^n = g^{mn} X_m Y_n = X^m Y_m \quad \dots (26)$$

Thus the scalar product depends only on the symmetric part of the tensor Z_{ij} , since $g_{mn} = g_{nm}$.

The vector product $[\mathbf{X}\mathbf{Y}]$ in three dimensions corresponds to the antisymmetric part of Z^{ij} according to the expression

$$\begin{aligned} [\mathbf{X}\mathbf{Y}]^r &= \epsilon^{rmn} X_m Y_n \\ [\mathbf{X}\mathbf{Y}]_r &= \epsilon_{rmn} X^m Y^n \end{aligned} \quad \dots (27)$$

or

in which

$$\left. \begin{aligned} \epsilon_{rst} &= \sqrt{g}; \quad \epsilon^{rst} = 1/\sqrt{g}; \\ &\quad rst \text{ cyclic permutation of } 123 \\ \epsilon_{rst} &= -\sqrt{g}; \quad \epsilon^{rst} = -1/\sqrt{g}; \\ &\quad rst \text{ cyclic permutation of } 321 \\ \epsilon_{rst} &= 0; \quad \epsilon^{rst} = 0; \\ &\quad \text{any two indices equal} \end{aligned} \right\} \quad \dots (28)$$

It is only in three dimensions that a vector product can be defined as a vector. In other spaces the skew symmetric part of the product tensor Z is referred to as the *outer product* of the two vectors. The symmetric part which defines the scalar product is called the *inner product*.

For convenience of reference Table 2.4.4 summarizes the principal properties of the base vectors and their reciprocals, and of the corresponding metric tensors. Examples in which some of these results are applied are given in 2.4.7.

† Not to be confused with the dyad of 2.4.5.

TABLE 2.4.4
Properties of Base and Reciprocal Systems

A. Scalar Products (Definitions)

$$(a_i a_j) = g_{ij}; (a^i a^j) = g^{ij}; (a^i a_j) = g^i_j$$

B. Transformations between Base and Reciprocal Vectors

$$a_i = g_{ij} a^j; a^i = g^{ij} a_j$$

C. Transformations between Base and Reciprocal Metric Tensors

NOTE. No summations are implied by double indices.

$$g g^{ij} = g_{ik} g_{kj} - g_{ij} g_{kk}; g g^{ii} = g_{jj} g_{kk} - (g_{jk})^2$$

$$g_{ij}/g = g^{ik} g^{kj} - g^{ij} g^{kk}; g_{ii}/g = g^{jj} g^{kk} - (g^{jk})^2$$

D. Vector Products in Base and Reciprocal Systems

$$[a_i a_j] = \sqrt{g} a^k; [a^i a^j] = a_k / \sqrt{g} \quad (i, j, k \text{ in cyclic order})$$

E. Mixed Vector Products

Note that $[a_i a^j] = -[a^j a_i]$.

Product	Components					
	a_1	a_2	a_3	a^1	a^2	a^3
$[a_1 a^1]$	0	$+g_{13}/\sqrt{g}$	$-g_{12}/\sqrt{g}$	0	$-g^{13}\sqrt{g}$	$+g^{12}\sqrt{g}$
$[a_1 a^2]$	$-g_{13}/\sqrt{g}$	0	$+g_{11}/\sqrt{g}$	0	$-g^{23}\sqrt{g}$	$+g^{22}\sqrt{g}$
$[a_1 a^3]$	$+g_{12}/\sqrt{g}$	$-g_{11}/\sqrt{g}$	0	0	$-g^{33}\sqrt{g}$	$+g^{32}\sqrt{g}$
$[a_2 a^1]$	0	$+g_{23}/\sqrt{g}$	$-g_{22}/\sqrt{g}$	$+g^{13}\sqrt{g}$	0	$-g^{11}\sqrt{g}$
$[a_2 a^2]$	$-g_{23}/\sqrt{g}$	0	$+g_{21}/\sqrt{g}$	$+g^{23}\sqrt{g}$	0	$-g^{21}\sqrt{g}$
$[a_2 a^3]$	$+g_{22}/\sqrt{g}$	$-g_{21}/\sqrt{g}$	0	$+g^{33}\sqrt{g}$	0	$-g^{31}\sqrt{g}$
$[a_3 a^1]$	0	$+g_{33}/\sqrt{g}$	$-g_{32}/\sqrt{g}$	$-g^{12}\sqrt{g}$	$+g^{11}\sqrt{g}$	0
$[a_3 a^2]$	$-g_{33}/\sqrt{g}$	0	$+g_{31}/\sqrt{g}$	$-g^{22}\sqrt{g}$	$+g^{21}\sqrt{g}$	0
$[a_3 a^3]$	$+g_{32}/\sqrt{g}$	$-g_{31}/\sqrt{g}$	0	$-g^{32}\sqrt{g}$	$+g^{31}\sqrt{g}$	0

2.4.5 Dyadics

A dyad is defined as a pair of vectors AB placed side by side without any sign of multiplication expressed or implied between them.† A *dyadic* Φ is the sum of any number of dyads, i.e.

$$\Phi = A_1 B_1 + A_2 B_2 + \dots + A_n B_n \quad \dots (1)$$

The first vector of any dyad is called the *antecedent*, the second vector the *consequent* of the dyad. The *conjugate* of Φ , i.e. Φ_C , is defined as

$$\Phi_C = B_1 A_1 + B_2 A_2 + \dots + B_n A_n \quad \dots (2)$$

Multiplication of a dyad by a scalar k is defined as the multiplication of either factor by k . A dyadic is multiplied by k when all its dyads are multiplied by k .

The product of the vector r with the dyadic Φ defined by

$$r \cdot \Phi = (r A_1) B_1 + (r A_2) B_2 + \dots + (r A_n) B_n = r_1 \quad \dots (3)$$

is called the *scalar product* of r with the dyadic, with r as *pre-factor* and Φ as *post-factor*. A second scalar product with Φ as pre-factor and r as post-factor is also defined, i.e.

$$\Phi \cdot r = A_1 (r B_1) + A_2 (r B_2) + \dots + A_n (r B_n) = r_2 \quad \dots (4)$$

It is now clear that

$$r_1 = r \cdot \Phi = \Phi_C \cdot r \quad \dots (5)$$

and of course that

$$r_2 = \Phi \cdot r = r \cdot \Phi_C \quad \dots (6)$$

It can be shown that any dyadic in three-dimensional space can be reduced to a form consisting of three dyads, and in this form the antecedents (consequents) can be three arbitrarily chosen non-coplanar vectors. In such a case the consequents (antecedents) completely determine the dyadic, i.e. the dyadic requires nine parameters for its specification.

If the antecedents and the consequents of a dyadic are both non-coplanar sets, the dyadic is said to be *complete*. If either the antecedents or the consequents are coplanar sets, the dyadic is said to be *planar* and can be reduced to two dyads, and if either the antecedents or the consequents are collinear, the dyadic is said to be *linear* and can be reduced to a single dyad.

In terms of any non-coplanar base triple a_i and its reciprocal triplet a^i (for notation see 2.4.4, page 54) any dyadic can be expressed in what is called the *nonion* form as the sum of nine dyads with appropriate numerical coefficients as follows:

$$\Phi = \phi_{ij} a^i a^j = \phi^{ij} a_i a_j = \phi^i_j a_i a^j = \phi_j^i a^i a_j \quad \dots (7)$$

in which summation over dummy indices is implied.

† Not to be confused with the general product of 2.4.4 (25).

The numerical coefficients of a dyadic in the nonion form are thus the components of a second order tensor in the corresponding covariant, contravariant or mixed forms (see 2.4.4, page 54).

The *scalar of a dyadic* is defined as

$$\Phi_S = (A_1 B_1) + (A_2 B_2) + \dots + (A_n B_n) = (\Phi_C)_S \dots (8a)$$

In terms of the coefficients of the nonion forms (7) the scalar can be written

$$\Phi_S = g^{ij} \phi_{ij} = g_{ij} \phi^{ij} = \phi^i_i = \phi_i^i \dots (8b)$$

in which g is the metric tensor.

The *vector of a dyadic* is defined as

$$\Phi_V = [A_1 B_1] + [A_2 B_2] + \dots + [A_n B_n] = -(\Phi_C)_V \dots (9a)$$

Using 2.4.4 (27), Φ_V may be written in terms of the nonion coefficients as

$$\Phi_V = \epsilon_{rpq} \phi^{pq} a^r = \epsilon^{rpq} \phi_{pq} a_r \dots (9b)$$

The *idemfactor* I is the dyadic which transforms every vector into itself, i.e.

$$r.I = I.r = r \dots (10)$$

The nonion forms for the idemfactor may be written

$$I = a^i a_i = a_i a^i = g^{ij} a_j a_i = g_{ij} a^i a^j \dots (11)$$

The *scalar product* $\Phi.\Psi$ of two dyadics is defined as follows.

If $s = r.\Phi$ and $t = s.\Psi$, then $t = r.(\Phi.\Psi)$. With

$$\Phi = \sum_i A_i B_i \quad \text{and} \quad \Psi = \sum_j C_j D_j$$

$$\text{then} \quad \Phi.\Psi = \sum_i \sum_j (B_i C_j) A_i D_j \dots (12)$$

and it follows that

$$I.\Phi = \Phi.I = \Phi \dots (13)$$

and that

$$(\Phi.\Psi)_C = \Psi_C.\Phi_C \dots (14)$$

The *vector product* of a vector with a dyadic is defined by

$$[r \times s].\Phi = r.[s \times \Phi] \dots (15a)$$

with

$$s \times \Phi = [s \times A_1] B_1 + [s \times A_2] B_2 + \dots + [s \times A_n] B_n \dots (15b)$$

If a dyadic is expressed in the trinomial form

$$\Phi = A_1 B_1 + A_2 B_2 + A_3 B_3$$

then the quantity

$$|\Phi| = (A_1 A_2 A_3)(B_1 B_2 B_3) \dots (16)$$

is called the *determinant of the dyadic*. If $|\Phi| \neq 0$ the dyadic is complete (non-singular). If $|\Phi| = 0$ the dyadic is planar or linear (singular). It may be shown that

$$|\Phi.\Psi| = |\Phi| |\Psi| \dots (17)$$

A dyadic is said to be *symmetric* if $\Phi = \Phi_C$, and it follows that $\Phi_V = 0$. It is *antisymmetric* if $\Phi = -\Phi_C$, and it follows that $\Phi_S = |\Phi| = 0$ and also that

$$\Phi = -\frac{1}{2} \Phi_V \times I = \frac{1}{2} I \times \Phi_V$$

If Φ is complete, the *reciprocal* Φ^{-1} is defined by

$$\Phi.\Phi^{-1} = \Phi^{-1}.\Phi = I \dots (18a)$$

and it follows that

$$(\Phi.\Psi)^{-1} = \Psi^{-1}.\Phi^{-1} \dots (18b)$$

One importance of dyadic notation for crystallography

TABLE 2.4.5

Dyadics for the Crystallographic Proper Rotations

NOTE. The dyadics for the corresponding improper rotations are obtained by changing all signs, i.e.

$$\begin{aligned} n &= uu + (I - uu) \cos 2\pi/n - I \times u \sin 2\pi/n & (n)_S &= 1 + 2 \cos 2\pi/n & (n)_V &= 2u \sin 2\pi/n \\ \bar{n} &= -uu - (I - uu) \cos 2\pi/n + I \times u \sin 2\pi/n & (\bar{n})_S &= -(1 + 2 \cos 2\pi/n) & (n)_V &= -2u \sin 2\pi/n \end{aligned}$$

n	General Dyadic	Nonion Form	Axial System	$(n)_S$	$(n)_V$
1	I	$I \equiv a^1 a_1 + a^2 a_2 + a^3 a_3$	Any axial system	3	0
2	$2uu - I$	$2 \equiv a^2 a_2 - a^3 a_3 - a^1 a_1$	$u = a_2/ a_2 $; $g_{12} = g_{23} = 0$	-1	0
3	$\frac{3}{2}uu - \frac{1}{2}I - \frac{\sqrt{3}}{2}I \times u$	$3 \equiv a^3 a_3 - a^2 a_2 + a^1 a_1 - a^2 a_1$ $3^{-1} \equiv a^3 a_3 - a^1 a_1 - a^1 a_2 + a^2 a_1$	$u = a_3/ a_3 $; $g_{11} = g_{22}$; $g_{23} = g_{31} = 0$; $g_{12} = -\frac{1}{2}$	0	$\sqrt{(3)}u$
		$3 \equiv a^1 a_2 + a^2 a_3 + a^3 a_1$ $3^2 \equiv a^2 a_1 + a^3 a_2 + a^1 a_3$	$u = (a_1 + a_2 + a_3)/ a_1 + a_2 + a_3 $; $g_{11} = g_{22} = g_{33}$; $g_{12} = g_{23} = g_{31}$		
4	$uu - I \times u$	$4 \equiv a^3 a_3 + a^1 a_2 - a^2 a_1$ $4^{-1} \equiv a^3 a_3 - a^1 a_2 + a^2 a_1$	$u = a_3/ a_3 $; $g_{11} = g_{22}$; $g_{12} = g_{23} = g_{31} = 0$	1	u
6	$\frac{1}{2}uu + \frac{1}{2}I - \frac{\sqrt{3}}{2}I \times u$	$6 \equiv a^3 a_3 + a^1 a_1 + a^1 a_2 - a^2 a_1$ $6^{-1} \equiv a^3 a_3 + a^2 a_2 - a^1 a_2 + a^2 a_1$	$u = a_3/ a_3 $; $g_{11} = g_{22}$; $g_{23} = g_{31} = 0$; $g_{12} = -\frac{1}{2}$	2	$\sqrt{(3)}u$

lies in the simple expression for the dyadics for rotations (proper or improper). For such dyadics

$$\Phi = \Phi_C^{-1}; |\Phi| = |\Phi_C| = \pm 1 \quad \dots (19a)$$

All such dyadics (post-factors) are of the form

$$\Phi = \pm \{uu + (I - uu) \cos \phi - I \times u \sin \phi\} \quad \dots (19b)$$

with

$$\Phi_S = \pm(1 + 2 \cos \phi) \quad \text{and} \quad \Phi_V = \pm 2 \sin \phi u \quad \dots (19c)$$

If $|\Phi| = +1$ the rotation is proper, if $|\Phi| = -1$ the rotation is improper.

Note that $u \cdot \Phi = \Phi \cdot u = \pm u$

and that therefore the vector u is invariant for a proper rotation and anti-invariant for an improper rotation. It is of course the rotation axis.

A complete derivation of point-group and space-group theory in terms of dyadic notation has been given by Zachariasen [40]. For convenience of reference his table for the five crystallographically possible rotations is reproduced (with slight modification to

conform to the conventions of these tables) as part of Table 2.4.5. Also included in this table are the nonion forms for these dyadics in terms of crystallographically customary co-ordinate systems.

2.4.6. Parallelism between Matrix, Tensor and Dyadic Notations for a Second Order Tensor

The transformation of the vector r into a vector s by means of a tensor A as pre-factor is represented in the dyadic notation by

$$s = A \cdot r \quad \dots (1)$$

The same tensor operating on r as a post-factor will produce a different vector

$$t = r \cdot A \quad \dots (2)$$

These two expressions provide a very convenient shorthand for the more complicated expressions which they represent. These more complicated expressions must, however, be used if detailed calculations are to

TABLE 2.4.6A

Comparison between Tensor, Dyadic and Matrix Notations

NOTE. In this table the parentheses do *not* denote scalar multiplication but merely group the terms of a vector or dyadic for clarity. The square brackets indicate matrices.

Tensor	Dyadic	Matrix
$s^i = A^{ij} r_j$ $s^i = A^i_j r^j$ $s_i = A_i^j r_j$ $s_i = A_{ij} r^j$	$s = A \cdot r$ $s = (A^{ij} a_i a_j) \cdot (r_k a^k)$ $s = (A^i_j a_i a^j) \cdot (r^k a_k)$ $s = (A_i^j a^i a_j) \cdot (r_k a^k)$ $s = (A_{ij} a^i a^j) \cdot (r^k a_k)$	$[s] = [A] [r]$ $[s^i] = [A^{ij}] [r_j]$ $[s^i] = [A^i_j] [r^j]$ $[s_i] = [A_i^j] [r_j]$ $[s_i] = [A_{ij}] [r^j]$
$t^j = r_i A^{ij}$ $t^j = r^i A_i^j$ $t_j = r_i A^i_j$ $t_j = r^i A_{ij}$	$t = r \cdot A$ $t = (r_k a^k) \cdot (A^{ij} a_i a_j)$ $t = (r^k a_k) \cdot (A_i^j a^i a_j)$ $t = (r_k a^k) \cdot (A^i_j a_i a^j)$ $t = (r^k a_k) \cdot (A_{ij} a^i a^j)$	$[t] = [r] [A]$ $[t^j] = [r_i] [A^{ij}]$ $[t^j] = [r^i] [A_i^j]$ $[t_j] = [r_i] [A^i_j]$ $[t_j] = [r^i] [A_{ij}]$

TABLE 2.4.6B

Matrix Transformations for Second Order Tensor

Transformations are written in tensor notation, but the order of the terms is correct for matrix multiplication if the first index is taken as the row index of the matrix and the second index as the column index.

	A^{ij}	A^i_j	A_i^j	A_{ij}
$A^{ij} =$	A^{ij}	$A^i_k g^{kj}$	$g^{ik} A_k^j$	$g^{ik} A_{km} g^{mj}$
$A^i_j =$	$A^{ik} g_{kj}$	A^i_j	$g^{ik} A_k^m g_{mj}$	$g^{ik} A_{kj}$
$A_i^j =$	$g_{ik} A^{kj}$	$g_{ik} A^k_m g^{mj}$	A_i^j	$A_{ik} g^{kj}$
$A_{ij} =$	$g_{ik} A^{km} g_{mj}$	$g_{ik} A^k_j$	$A_i^k g_{kj}$	A_{ij}

be carried out. The vector \mathbf{r} must be expressed in terms of the base triple or its reciprocal triple as in equations 2.4.4 (1a) or (6a) and the dyadic \mathbf{A} in one of its four nonion forms (2.4.5 (7)). The expanded expressions are then those shown in column 2 of Table 2.4.6A. In column 1 of the same table the corresponding tensor expressions are shown, and the equivalent matrix expressions are shown in column 3. If now we reduce the products of column 2 by means of the defining equations of the reciprocal triple (cf. 2.4.3.2), i.e.

$$(\mathbf{a}^i \mathbf{a}_j) = \delta^i_j \quad \dots (3)$$

we see that all three notations reduce to exactly the same calculation, a matrix multiplication.

Table 2.4.6B shows the transformations which relate the four forms (cf. 2.4.4 (8) and (9)) in which the components of a second order tensor may be expressed. The one table serves for both the tensor and matrix notations. The reader may easily rewrite this table in dyadic form by accompanying each tensor by its nonion dyad (cf. 2.4.5 (7)) and applying dot multiplication to the resulting expressions.

2.4.7. Vector and Tensor Problems in Crystal Analysis

In the present section several problems of importance in crystal structure work are selected as examples of the methods described in the preceding sections of

2.4. No attempt has been made to indicate all the problems which will be encountered, nor has any attempt been made to adhere exclusively to one notation. In each case it should be apparent to the reader how a problem written out in tensor notation, for example, can be rewritten in dyadic or in matrix form.

2.4.7.1. CALCULATIONS OF BOND LENGTHS AND BOND ANGLES

An atom ${}_sP$ is located in the cell by the contravariant components ${}_s x^i$ of the vector from the origin to the atomic position. Here the prefixed subscript simply indicates the number of the atom, while the suffixed superscript indicates the number of the contravariant component. The vector from the origin is

$${}_s \mathbf{r} = {}_s x^1 \mathbf{a}_1 + {}_s x^2 \mathbf{a}_2 + {}_s x^3 \mathbf{a}_3 \quad \dots (1)$$

These contravariant components are simply the fractional co-ordinates usually used in crystallography.

In these terms, the distance

$${}_s t \mathbf{r} = {}_t \mathbf{r} - {}_s \mathbf{r} \quad \dots (2)$$

has a magnitude ${}_s t r$ which may be calculated from 2.4.4 (15), i.e.

$${}_s t r^2 = g_{ij} {}_s t \delta^i {}_s t \delta^j \quad \dots (3)$$

in which

$${}_s t \delta^i = {}_t x^i - {}_s x^i \quad \dots (4)$$

The angle ϕ_{tsu} at the atom ${}_sP$ between the vectors

TABLE 2.4.7A
Metric Tensors for Crystal Lattices

Lattices	g_{ii}	g_{ij}	g^{ii}	g^{ij}
Triclinic ..	a_i^2	$a_i a_j \cos \alpha_k$	$(a^i)^2$ (see NOTE)	$a^i a^j \cos \alpha^k$
Monoclinic .. \mathbf{a}_i unique	a_i^2	$g_{ij} = g_{ki} = 0$ $g_{jk} = a_j a_k \cos \alpha_i$	$(a^i)^2$	$g^{ij} = g^{ki} = 0$ $g^{jk} = a^j a^k \cos \alpha^i$
Orthorhombic	a_i^2	0	$1/(a_i)^2$	0
Tetragonal .. \mathbf{a}_3 unique	$g_{11} = g_{22} = a^2$ $g_{33} = c^2$	0	$g^{11} = g^{22} = 1/a^2$ $g^{33} = 1/c^2$	0
Rhombohedral	$g_{11} = g_{22} = g_{33} = a^2$	$g_{12} = g_{23} = g_{31} = a^2 \cos \alpha$	$g^{11} = g^{22} = g^{33} =$ $\frac{1 + \cos \alpha}{a^2(1 - \cos \alpha)(1 + 2 \cos \alpha)}$	$g^{12} = g^{23} = g^{31} =$ $\frac{- \cos \alpha}{a^2(1 - \cos \alpha)(1 + 2 \cos \alpha)}$
Hexagonal .. \mathbf{a}_3 unique	$g_{11} = g_{22} = a^2$ $g_{33} = c^2$	$g_{23} = g_{31} = 0$ $g_{12} = -\frac{1}{2}a^2$	$g^{11} = g^{22} = 4/3a^2$ $g^{33} = 1/c^2$	$g^{23} = g^{31} = 0$ $g^{12} = 2/3a^2$
Cubic	$g_{11} = g_{22} = g_{33} = a^2$	0	$g^{11} = g^{22} = g^{33} = 1/a^2$	0

NOTE. The contravariant components of the metric tensors are given in terms of the reciprocal lattice parameters for the triclinic and monoclinic systems. They can be calculated in terms of the base system parameters by the formulae of Table 2.4.4C. The contravariant components for all other lattices are given in terms of the base system parameters.

joining it to the atoms tP and uP is then given by 2.4.4 (16), i.e.

$$st\mathbf{r}_{su}\mathbf{r} \cos \phi_{tsu} = g_{ij} \delta^i_{st} \delta^j_{su} \quad \dots (5)$$

The matrices g_{ij} needed for these calculations are given in Table 2.4.7A for the seven primitive lattices.

It is clear that the detailed expansions of (3) and (5) are very cumbersome for the triclinic and the rhombohedral cases, and are only a little less difficult to handle for the cases in which there is only one general cell angle (monoclinic and hexagonal). It is only in the orthogonal systems that formulae (3) and (5) are practical if a large number of distances and angles are to be calculated. Of course, if only one or two distances or angles are to be calculated these formulae probably offer the best method.

If many such calculations are to be carried out there are two approaches. In the first, the covariant components of all vectors (e.g. ${}_s x_i$) are calculated by 2.4.4 (21), i.e.

$${}_s x_i = g_{ij} ({}_s x^j) \quad \dots (6)$$

The formula (3) then takes the simple form

$$st\mathbf{r}^2 = {}_{st} \delta^i_{st} \delta_i \quad \dots (7)$$

and (5) becomes

$$st\mathbf{r}_{su}\mathbf{r} \cos \phi_{tsu} = {}_{st} \delta^i_{su} \delta_i \quad \dots (8)$$

These formulae are much simpler than (3) and (5) for the non-orthogonal systems, and it may be that they will be of use for machine calculations.

The second of the two approaches mentioned above involves the transformation of all quantities to an orthonormal system. For example, one might choose an axis A_1 of unit length in the direction of \mathbf{a}_1 , a second axis A_2 perpendicular to \mathbf{a}_1 and in the plane of \mathbf{a}_1 and \mathbf{a}_2 , and an axis A_3 perpendicular to that plane. Thus we set

$$\left. \begin{aligned} A_1 &= \mathbf{a}_1 / |\mathbf{a}_1| \\ A_2 &= \mathbf{a}_3 \times \mathbf{a}_1 \\ A_3 &= \mathbf{a}^3 / |\mathbf{a}^3| \end{aligned} \right\} \quad \dots (9)$$

and by using the results of Table 2.4.4E and 2.4.4 (20) we may write $[A_i] = [\alpha_i^j][a_j]$ (cf. 2.4.4, page 54).

$$\left. \begin{aligned} A_1 &= \mathbf{a}_1 / \sqrt{g_{11}} \\ A_2 &= -g_{12}\mathbf{a}_1 / \sqrt{(g_{11}g^{33}) + (g_{11}/g^{33})\mathbf{a}_2} \\ A_3 &= g^{31}\mathbf{a}_1 / \sqrt{g^{33} + g^{32}\mathbf{a}_2 / \sqrt{g^{33} + (\sqrt{g^{33}})\mathbf{a}_3}} \end{aligned} \right\} \quad \dots (10)$$

and its inverse

$$[a_i] = [\beta_i^j][A_j]$$

$$\left. \begin{aligned} \mathbf{a}_1 &= (\sqrt{g_{11}})A_1 \\ \mathbf{a}_2 &= g_{12}A_1 / \sqrt{g_{11}} + \sqrt{(g_{11}g^{33})/g_{11}}A_2 \\ \mathbf{a}_3 &= g_{31}A_1 / \sqrt{g_{11}} - (\sqrt{g_{11}})g^{32}A_2 / \sqrt{(g_{11}g^{33})} + A_3 / \sqrt{g^{33}} \end{aligned} \right\} \quad \dots (11)$$

The corresponding transformations for the contravariant components are then written down directly as $[X^i] = [x^j][\beta_j^i]$ (cf. 2.4.4 (5), etc.), i.e.

$$\left. \begin{aligned} X^1 &= (\sqrt{g_{11}})x^1 + g_{12}x^2 / \sqrt{g_{11}} + g_{31}x^3 / \sqrt{g_{11}} \\ X^2 &= \sqrt{(g_{11}g^{33})/g_{11}}x^2 - (\sqrt{g_{11}})g^{32}x^3 / \sqrt{(g_{11}g^{33})} \\ X^3 &= x^3 / \sqrt{g^{33}} \end{aligned} \right\} \quad \dots (12)$$

and its inverse $[x^i] = [X^j][\alpha_j^i]$, i.e.

$$\left. \begin{aligned} x^1 &= X^1 / \sqrt{g_{11}} - g_{12}X^2 / \sqrt{(g_{11}g^{33})} + g^{31}X^3 / \sqrt{g^{33}} \\ x^2 &= \sqrt{(g_{11}g^{33})}X^2 + g^{32}X^3 / \sqrt{g^{33}} \\ x^3 &= (\sqrt{g^{33}})X^3 \end{aligned} \right\} \quad \dots (13)$$

In the transformed system the usual methods of analytic geometry can then be applied. The numerical procedure for such a calculation is quite parallel to that given for the monoclinic case in the following Section.

2.4.7.2. NUMERICAL EXAMPLE OF THE CALCULATION OF BOND LENGTHS AND BOND ANGLES

The calculation for a monoclinic lattice is given here for the sake of brevity. It differs from that for a triclinic lattice only in its complication but not in principle. Unit vectors A and B are chosen parallel to \mathbf{a} and \mathbf{b} respectively, and the third vector C is perpendicular to the first two. We have clearly

$$\begin{aligned} \mathbf{a} &= aA \\ \mathbf{b} &= bB \\ \mathbf{c} &= c \cos \beta A + c \sin \beta C \end{aligned}$$

This transformation may be written formally $[\mathbf{a}] = [\beta][A]$ (cf. 2.4.4 (2b)), since $[\mathbf{a}]$ and $[A]$ are of course covariant. We then have

$$[\beta] = \begin{bmatrix} a & 0 & 0 \\ 0 & b & 0 \\ c \cos \beta & 0 & c \sin \beta \end{bmatrix} \quad \dots (14a)$$

The determinant of this matrix is equal to the volume of the cell $V = abc \sin \beta$. The inverse of this matrix is

$$[\alpha] = \begin{bmatrix} 1/a & 0 & 0 \\ 0 & 1/b & 0 \\ -1/(a \tan \beta) & 0 & 1/(c \sin \beta) \end{bmatrix} \quad \dots (14b)$$

and in these two matrices (cf. 2.4.4) we have all the information necessary to effect transformations of vectors or tensors from one system to the other.

EXAMPLE

In a particular case

$a = 12.792 \text{ \AA}$ $b = 5.627 \text{ \AA}$ $c = 11.474 \text{ \AA}$ and $\beta = 111.17^\circ$ and we have $\sin \beta = 0.932513$ and $\cos \beta = -0.361136$. The two matrices are then†

$$[\beta] = \begin{bmatrix} 12.79200 & 0 & 0 \\ 0 & 5.62700 & 0 \\ -4.14368 & 0 & 10.69965 \end{bmatrix} (\text{\AA}) \quad \dots (15a)$$

and its inverse

$$[\alpha] = \begin{bmatrix} 0.0781739 & 0 & 0 \\ 0 & 0.1777146 & 0 \\ 0.0302746 & 0 & 0.0934610 \end{bmatrix} (\text{\AA}^{-1}) \quad \dots (15b)$$

In this problem we are interested in calculating the

† We have calculated these matrices in \AA since we are almost exclusively concerned with the matrix $[\alpha]$. It is usually preferable to use millimicrons ($1 \text{ m}\mu = 10 \text{ \AA}$) as units in such calculations in order that the coefficients of the two matrices are more nearly of the same magnitude. To avoid rounding errors in matrix calculations it is wise to carry several figures beyond the accuracy justified by the data.

2.4. VECTOR AND TENSOR ANALYSIS

bond lengths and bond angles in a carboxyl group in which C_6 is the carboxyl carbon and C_3 the carbon to which it is joined. O_5 and O_6 are the carboxyl oxygens. The fractional co-ordinates x, y, z are transformed

into the Cartesian co-ordinates X, Y, Z by the contra-variant transformation $[X] = [x][\beta]$ (cf. 2.4.4 (5) and 2.4.7.1 (11) and (12)). The two sets of co-ordinates are tabulated as follows:

	x	y	z	X	Y	Z
C_6	0.0458	0.1332	0.1684	-0.11192	0.74952	1.80182
O_5	0.0142	0.2722	0.0682	-0.10095	1.53167	0.72972
O_6	-0.0113	-0.0249	0.1849	-0.91072	-0.14011	1.97837
C_3	0.1627	0.1955	0.2616	0.99727	1.10008	2.79903

The vectors from C_6 to the other three atoms are then investigated (in terms of the Cartesian system) in the following table:

	Co-ordinate Differences			Bond Lengths		Direction Cosines		
	ΔX	ΔY	ΔZ	r^2	r	l	m	n
C_6-O_5	0.01097	0.78215	-1.07210	1.76127	1.32713	0.008266	0.589354	-0.807833
C_6-O_6	-0.79880	-0.88963	0.17655	1.46069	1.20859	-0.660935	-0.736089	0.146079
C_6-C_3	1.10919	0.35056	0.99721	2.34762	1.53219	0.723925	0.228797	0.650840

From the direction cosines of the last three columns, the bond angles ϕ can be calculated directly from the scalar products of the pairs of vectors as follows:

	Bond Angles		Direction Cosines of Vector Product		
	$\cos \phi$	ϕ	l	m	n
$O_5C_6O_6$	-0.557288	123.87°	-0.612468	0.641581	0.461798
$O_6C_6C_3$	-0.551808	123.49°	-0.614524	0.642600	0.457630
$O_5C_6C_3$	-0.384944	112.64°	-0.615860	0.639464	0.460219
		360.00°			

In the same table are included the direction cosines of the vector products of the three pairs of vectors. These are very close to parallel, as was suggested by the fact that the three angles added up to 360.00° (a fortuitous accuracy), indicating that all four atoms are very close to coplanar. An average of these three vectors (normalized) gives the vector: -0.614286; 0.641217; 0.459884, which must be very close to the unit normal to the plane most nearly containing all four atoms. This vector is (HKL) for the plane in question, and if one is interested in the corresponding Miller indices one must use the corresponding transformation for covariant components, i.e. $[h] = [\beta][H]$ (cf. 2.4.4 (7)),

and one obtains the vector: -7.8579; 3.6081; 7.4660. This is of course quite close to the $(\bar{2}12)$ plane.

These are only a few of the calculations which can readily be carried out in Cartesian space and for which the results can immediately be reconverted to the non-orthogonal system.

2.4.7.3. ROTATIONS

In a Cartesian system (2.4.3.3, page 53) the point $[y^i]$ is rotated to the point $[Y^i]$ by the operation of the matrix $[\rho]$ on the row symbols as post-multiplier, i.e.

$$[Y^i] = [y^i][\rho] \quad \dots(16)$$

where

$$[\rho] = \begin{bmatrix} \cos \alpha + l_1^2(1 - \cos \alpha) & l_1 l_2(1 - \cos \alpha) + l_3 \sin \alpha \\ l_1 l_2(1 - \cos \alpha) - l_3 \sin \alpha & \cos \alpha + l_2^2(1 - \cos \alpha) \\ l_3 l_1(1 - \cos \alpha) + l_2 \sin \alpha & l_2 l_3(1 - \cos \alpha) - l_1 \sin \alpha \\ l_3 l_1(1 - \cos \alpha) - l_2 \sin \alpha & l_2 l_3(1 - \cos \alpha) + l_1 \sin \alpha \\ \cos \alpha + l_3^2(1 - \cos \alpha) & \end{bmatrix} \dots (17)$$

in which $l_1 l_2 l_3$ are the Cartesian direction cosines of the rotation axis and α is the angle of rotation about that axis. The special forms of $[\rho]$ for the crystallographic axes are listed in Table 2.4.7B.

If we wish to calculate the rotation matrix $[\mathbf{P}]$ which describes the same rotation in an oblique system $[x^i]$, $[X^i]$, i.e.

$$[X^i] = [x^i][\mathbf{P}] \dots (18)$$

we make use of 2.4.4(5) and write

$$[X^i] = [Y^i][\alpha] \quad \text{and} \quad [y^i] = [x^i][\beta]$$

in (16) and obtain

$$[X^i] = [Y^i][\alpha] = [y^i][\rho][\alpha] = [x^i][\beta][\rho][\alpha] = [x^i][\mathbf{P}] \dots (19)$$

We find that

$$[\mathbf{P}] = [\beta][\rho][\alpha] \dots (20)$$

If we wish to find the matrix $[\mathbf{P}]$ for hexagonal and trigonal axes in a hexagonal co-ordinate system $[x^i]$, we first recognize that

$$\begin{aligned} e_1 &= a_1/a_1 \\ e_2 &= \left(\frac{1}{\sqrt{3}}a_1 + \frac{2}{\sqrt{3}}a_2 \right) / a_1 \\ e_3 &= a_3/a_3 \end{aligned} \dots (21)$$

is a unit vector system for the Cartesian co-ordinates $[y^i]$ and thus by 2.4.4(2) we have

$$[\alpha] = \begin{bmatrix} 1/a_1 & 0 & 0 \\ 1/(a_1\sqrt{3}) & 2/(a_1\sqrt{3}) & 0 \\ 0 & 0 & 1/a_3 \end{bmatrix} \dots (22a)$$

and its inverse

$$[\beta] = \begin{bmatrix} a_1 & 0 & 0 \\ -\frac{1}{2}a_1 & (\sqrt{3})a_1/2 & 0 \\ 0 & 0 & a_3 \end{bmatrix} \dots (22b)$$

The rotation matrices $[\rho]$ for the operations 3 and 6

TABLE 2.4.7B
Cartesian Rotation Matrices for the Crystallographic Axes

Note that the inverses of these matrices are their transposes and that the matrices for \bar{n} are obtained by changing the signs of all terms in the matrices for n .

n	$\cos \alpha$	$\sin \alpha$	Matrix for $[l_1 l_2 l_3]$	Important special cases	
1	1	0	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$		
2	-1	0	$\begin{bmatrix} 2l_1^2-1 & 2l_1l_2 & 2l_3l_1 \\ 2l_1l_2 & 2l_2^2-1 & 2l_2l_3 \\ 2l_3l_1 & 2l_2l_3 & 2l_3^2-1 \end{bmatrix}$	$[001] \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	$[110] \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$
3	$-\frac{1}{2}$	$\frac{\sqrt{3}}{2}$	$\begin{bmatrix} \frac{1}{2}(3l_1^2-1) & \frac{1}{2}\{3l_1l_2+(\sqrt{3})l_3\} & \frac{1}{2}\{3l_3l_1-(\sqrt{3})l_2\} \\ \frac{1}{2}\{3l_1l_2-(\sqrt{3})l_3\} & \frac{1}{2}(3l_2^2-1) & \frac{1}{2}\{3l_2l_3+(\sqrt{3})l_1\} \\ \frac{1}{2}\{3l_3l_1+(\sqrt{3})l_2\} & \frac{1}{2}\{3l_2l_3-(\sqrt{3})l_1\} & \frac{1}{2}(3l_3^2-1) \end{bmatrix}$	$[001] \begin{bmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}$	$[111] \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$
4	0	1	$\begin{bmatrix} l_1^2 & l_1l_2+l_3 & l_3l_1-l_2 \\ l_1l_2-l_3 & l_2^2 & l_2l_3+l_1 \\ l_3l_1+l_2 & l_2l_3-l_1 & l_3^2 \end{bmatrix}$	$[001] \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	
6	$\frac{1}{2}$	$\frac{\sqrt{3}}{2}$	$\begin{bmatrix} \frac{1}{2}(l_1^2+1) & \frac{1}{2}\{l_1l_2+(\sqrt{3})l_3\} & \frac{1}{2}\{l_3l_1-(\sqrt{3})l_2\} \\ \frac{1}{2}\{l_1l_2-(\sqrt{3})l_3\} & \frac{1}{2}(l_2^2+1) & \frac{1}{2}\{l_2l_3+(\sqrt{3})l_1\} \\ \frac{1}{2}\{l_3l_1+(\sqrt{3})l_2\} & \frac{1}{2}\{l_2l_3-(\sqrt{3})l_1\} & \frac{1}{2}(l_3^2+1) \end{bmatrix}$	$[001] \begin{bmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}$	

about a Cartesian axis [001] can both be represented by the matrix

$$[\rho] = \begin{bmatrix} \frac{1}{2}s & (\sqrt{3})/2 & 0 \\ -(\sqrt{3})/2 & \frac{1}{2}s & 0 \\ 0 & 0 & 1 \end{bmatrix} \dots (23)$$

in which $s=-1$ for the operation 3 and $+1$ for the operation 6. The corresponding matrices $[\mathbf{P}]$ are then given by (20).

$$[\mathbf{P}] = [\beta][\rho][\alpha] = \begin{bmatrix} \frac{1}{2}(s+1) & 1 & 0 \\ -1 & \frac{1}{2}(s-1) & 0 \\ 0 & 0 & 1 \end{bmatrix} \dots (24)$$

and the matrices for the two operators are specifically

$$\mathbf{3} \equiv \begin{bmatrix} 0 & 1 & 0 \\ -1 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \text{and} \quad \mathbf{6} \equiv \begin{bmatrix} 1 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \dots (25)$$

with their inverses

$$\mathbf{3}^{-1} \equiv \begin{bmatrix} -1 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \text{and} \quad \mathbf{6}^{-1} \equiv \begin{bmatrix} 0 & -1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \dots (26)$$

It is well to remind the reader that covariant quantities are transformed as post-factors by the inverse matrix (cf. 2.4.4(5) and (7) and the related text). Thus, to be specific, the operation 3 transforms the coordinates x^1, x^2, x^3 into $-x^2, x^1-x^2, x^3$, while the same operation transforms the indices $h_1 h_2 h_3$ into $-(h_1+h_2), h_1, h_3$.

For discussions of vector analysis see almost any textbook of theoretical physics and also [4], page 132 *et seq.* For general references in relation to Section 2.4 see [35]–[40].

2.5. Fourier Theory

In the following discussion the need for brevity will not permit complete mathematical rigour in the statement of results. Mathematical limitations are included only when they are of importance in the understanding of the results or in the efficiency of their application to crystallographic theory. Almost every textbook of theoretical physics contains a brief treatment of Fourier analysis.

2.5.1. Orthogonal Functions

A set of functions $\psi_n(x)$ of a real variable x is said to form an *orthogonal set of functions for the range* $a < x < b$ if

$$[N_n N_m (b-a)]^{-1} \int_a^b \psi_n(x) \tilde{\psi}_m(x) dx = \delta_{nm} \quad \dots (1)$$

where δ_{mn} is the Kronecker delta defined by

$$\delta_{mn} = 0 (m \neq n); = 1 (m = n) \quad \dots (2)$$

The functions $\psi_n(x)$ are said to form an *orthonormal set* for the interval if for every n the *normalization factor* N_n defined by

$$[b-a]^{-1} \int_a^b |\psi_n(x)|^2 dx = N_n^2 \quad \dots (3)$$

has the value unity.

A function $f(x)$ defined at every point within the specified range has a representation in terms of an orthonormal set in ψ_n by the Fourier† series or *orthonormal series*.

$$f(x) = \sum_n a_n \psi_n(x) \quad \dots (4a)$$

where
$$a_n = [(b-a)]^{-1} \int_a^b f(x) \tilde{\psi}_n(x) dx \quad \dots (4b)$$

The set of constants a_n are called the *Fourier constants* of the function $f(x)$ with respect to the set ψ_n . These constants as defined by (4b) have the property of minimizing the mean square deviation of any number of terms of the series (4a) from the function $f(x)$. This minimum deviation is

$$\begin{aligned} [b-a]^{-1} \int_a^b |f(x) - \sum_n a_n \psi_n(x)|^2 dx \\ = [b-a]^{-1} \int_a^b |f(x)|^2 dx - \sum_n |a_n|^2 \quad \dots (5) \end{aligned}$$

The Fourier representation of a given function $f(x)$ (i.e. the series 4a) is the closest approximation in the least squares sense which can be achieved by means of an arbitrarily selected set of the orthonormal functions

ψ_n . This does not mean that the approximation is “close” in any sense other than that of the least squares theory. See for example the discussion of Gibbs phenomenon in [41]. Expression (5) is known as *Bessel’s formula*, and from (5) we clearly have *Bessel’s inequality*

$$\sum_n |a_n|^2 \leq [b-a]^{-1} \int_a^b |f(x)|^2 dx \quad \dots (6)$$

If the equality sign in (6) is valid, this expression is known as *Parseval’s equation*.

If Parseval’s equation is true for the expansions of all functions belonging to a certain class in terms of a certain set of orthonormal functions, that set of orthonormal functions is said to be *complete* with respect to that class of functions and the expansion (4) will be *unique*.

A detailed discussion of the nature of the convergence of Fourier series is beyond our scope. It is sufficient to say that if the integral on the right of (6) is finite and if $f(x)$ has a finite number of discontinuities, the Fourier series with respect to a complete set ψ_n will converge to $f(x)$ everywhere except at the discontinuities. At these points the series is not convergent in the usual sense but is summable to the value

$$\lim_{\epsilon \rightarrow 0} \frac{1}{2} \{f(x+\epsilon) + f(x-\epsilon)\} \quad \dots (7)$$

The most important orthogonal set from the crystallographer’s point of view is the set $e^{2\pi i n x}$, where n is any integer, positive, negative or zero. The set is clearly orthonormal for the range $0 < x < 1$, and complete, and expansions in terms of this set will be periodic with period unity. Such series are of course the Fourier series discussed in 2.5.4, page 73.

The set of functions $\sqrt{2} \cos 2\pi n x$, $\sqrt{2} \sin 2\pi n x$, together with the constant 1 also forms an orthonormal set for the range $0 < x < 1$ and leads to an alternative presentation of Fourier series.

The detailed discussion of the orthogonality of the non-denumerable set $e^{2\pi i u x}$ where u is not restricted to integers in the range $-\infty < u < \infty$ is beyond our scope here. Reference must be made to texts on the Fourier integral theorem.

A second orthogonal set of importance to the theory of Fourier transforms is provided by the set of Hermite functions $\phi_n(\alpha x)$, where n is a positive integer or zero and α is an arbitrary parameter. As is often the case

† Mathematicians are inclined to use the term Fourier Series for all expansions in terms of orthogonal or orthonormal functions. We shall confine the term Fourier Series in later sections to the usual usage in terms of $e^{2\pi i n x}$ or the corresponding cosine or sine series and use the terms *orthonormal series* or *orthogonal series* for expansions in terms of other functions, but for the present section it will be more convenient to continue the mathematician’s usage.

with orthogonal sets, these functions can be defined by a *generating function*[†]

$$T(x, t) = e^{\alpha^2 x^2 / 2 - (\alpha x - t)^2} = \sum_{n=0}^{\infty} N_n \phi_n(\alpha x) t^n / n! \quad \dots (8)$$

Using this definition it is now easy to show that the functions $\phi_n(\alpha x)$ form an orthonormal set[‡] over the range $-\infty < x < \infty$. This is done by integrating the product $T(x, s)T(x, t)$ with respect to x over the doubly infinite range and expanding the resulting series in comparison with the integral of the double series representation of the product. It follows that the $\phi_n(\alpha x)$ are orthonormal over the range, provided that

$$N_n = \left[\frac{\sqrt{\pi}}{\alpha} 2^n n! \right]^{-1/2} \quad \dots (9)$$

By calculating the Fourier transform of (8) with respect to x (see 2.5.3) it is easy to show that

$$(i)^n \phi_n\{\sqrt{(2\pi)u}\} = \int \phi_n\{\sqrt{(2\pi)x}\} e^{2\pi i u x} dx \quad \dots (10)$$

The first few Hermite functions are given explicitly by

$$\begin{aligned} N_0 \phi_0(\alpha x) &= e^{-\alpha^2 x^2 / 2} & N_0^2 &= (\sqrt{\pi}) / \alpha \\ N_1 \phi_1(\alpha x) &= 2\alpha x e^{-\alpha^2 x^2 / 2} & N_1^2 &= 2(\sqrt{\pi}) / \alpha \\ N_2 \phi_2(\alpha x) &= 2(2\alpha^2 x^2 - 1) e^{-\alpha^2 x^2 / 2} & N_2^2 &= 8(\sqrt{\pi}) / \alpha \\ N_3 \phi_3(\alpha x) &= 4(2\alpha^3 x^3 - 3\alpha x) e^{-\alpha^2 x^2 / 2} & N_3^2 &= 48(\sqrt{\pi}) / \alpha \end{aligned} \quad \dots (11)$$

or more generally

$$N_n \phi_n(\alpha x) = \left(\frac{\partial^n T}{\partial t^n} \right)_{t=0} \quad \dots (12)$$

Note that $\phi_n(x)$ defined here differs from that defined by Campbell and Foster [63]. The latter is

$$(-1)^n (2\pi)^{n/2} N_n \phi_n\{\sqrt{(2\pi)x}\}$$

in our notation. Our definition agrees with that of Courant-Hilbert, Wiener, Titchmarsh [50], etc.

2.5.2. The Delta Function

Consider the function

$$D(x, \alpha) = \frac{1}{\alpha} e^{-\pi x^2 / \alpha^2} \quad \dots (1a)$$

and its infinite integral

$$\int_{-\infty}^{\infty} D(x, \alpha) dx = 1 \quad \dots (1b)$$

Thus the area under the curve D plotted as a function of x has a constant value unity irrespective of the value of α . At $x=0$ the value of D tends to infinity as α tends to 0, while for $x \neq 0$, the value of D tends to zero as α tends to zero.

Thus if we define

$$\delta(x) = \lim_{\alpha \rightarrow 0} \frac{1}{\alpha} e^{-\pi x^2 / \alpha^2} \quad \dots (2)$$

we shall have Dirac's *delta function*, for which

$$\begin{aligned} \delta(x) &= 0; \quad x \neq 0 \\ &= \infty; \quad x = 0 \end{aligned} \quad \int_{-\infty}^{\infty} \delta(x) dx = 1 \quad \dots (3)$$

The important properties of $\delta(x)$ are as follows:

$$\int_{-\infty}^{\infty} f(x) \delta(x - x_0) dx = f(x_0) \quad \dots (4)$$

and in particular

$$\int_{-\infty}^{\infty} \delta(x) \delta(x - x_0) dx = \delta(x_0) \quad \dots (5)$$

$$\text{and} \quad \int_{-\infty}^{\infty} e^{\pm 2\pi i u x} \delta(x - x_0) dx = e^{\pm 2\pi i u x_0} \quad \dots (6)$$

Note that in (3)–(6) the range of integration need not be doubly infinite, but need only include the value x_0 at which the delta function is non-zero.

The delta function may be defined otherwise than above. Thus we may write

$$\delta_1(x) = \lim_{N \rightarrow \infty} \frac{\sin \pi N x}{\pi x} \quad \dots (7)$$

Here we cannot say that (at $x \neq 0$) $\delta_1(x)$ equals zero in the limit. It oscillates with infinite frequency between $\pm 1/\pi x$, and will thus make zero contribution to any integral of the types (3)–(6).

The delta function is a special case \mathcal{S}_0 of the singularity functions \mathcal{S}_n defined by Campbell and Foster [63].

In n dimensions the delta function is defined by

$$\delta(\mathbf{x}) = \lim_{\alpha \rightarrow 0} \frac{1}{\alpha^n} e^{-\frac{\pi}{\alpha^2} \sum_{i=1}^n x_i^2} \quad \dots (8)$$

The results (3)–(6) then hold for the corresponding multiple integrals.

2.5.3. Fourier Transforms

Although historically the notion of Fourier transforms arose from the theory of Fourier series, it is profitable as far as crystallography is concerned to consider Fourier transforms first.

2.5.3.1. BASIC MATHEMATICS

The function $F(u)$ defined by the integral equation

$$f(x) = \int_{-\infty}^{\infty} F(u) e^{-2\pi i u x} du \quad \dots (1a)$$

is called the *Fourier transform* of $f(x)$ and is given by

$$F(u) = \int_{-\infty}^{\infty} f(x) e^{2\pi i u x} dx \quad \dots (1b)$$

[†] Details of other orthogonal sets and of their generating functions and other properties are given in many places, for example [53].

[‡] In working with an infinite range the factor $[b-a]^{-1}$ must be replaced by unity in the above treatment of the orthonormal set.

Symbolically, we write

$$F(u) = T[f(x)] \quad \dots (2a)$$

and $f(x) = T^{-1}[F(u)] \quad \dots (2b)$

By the operation T we mean multiplication by the kernel $e^{2\pi i u x}$ and integration with respect to the variable x or u contained in the operand; and by T^{-1} we mean the same operation with the kernel $e^{-2\pi i u x}$. Thus

$$T^2[f(x)] = f(-x) = T[F(u)], \text{ etc.} \quad \dots (3)$$

The operator T forms a group of order four. Note that the formulae (1) are not completely symmetrical. They do exhibit many important symmetry properties which are of great value, but neglect of the change of sign in the kernel can lead to considerable trouble.

The *Fourier cosine transform* $F_c(u)$ of $f(x)$ for the range $0 \leq x < \infty$ is defined by

$$f(x) = 2 \int_0^\infty F_c(u) \cos 2\pi u x \, du \quad \dots (4a)$$

and $F_c(u) = 2 \int_0^\infty f(x) \cos 2\pi u x \, dx \quad \dots (4b)$

The *Fourier sine transform* $F_s(u)$ of $f(x)$ for the range $0 \leq x < \infty$ is defined similarly by

$$f(x) = 2 \int_0^\infty F_s(u) \sin 2\pi u x \, du \quad \dots (5a)$$

and $F_s(u) = 2 \int_0^\infty f(x) \sin 2\pi u x \, dx \quad \dots (5b)$

We shall make no further use of the cosine and sine transforms except to note the useful fact that for *even* functions $f(x)$

$$F(u) = F_c(u) \quad \dots (6a)$$

and for *odd* functions $f(x)$

$$F(u) = iF_s(u) \quad \dots (6b)$$

Thus the expressions (5) and (6) are often of help in evaluating Fourier transforms as defined by (1).

If $f(x)$ is a *real function* of x , it is clear that

$$F(u) = \tilde{F}(-u) \quad \dots (7)$$

and that the real part of $F(u)$ is even and depends only on the even part of $f(x)$, while the imaginary part of $F(u)$ is odd and depends only on the odd part of $f(x)$.

The *characteristic functions* of the Fourier transform are those functions which are a constant multiple of their own Fourier transforms, i.e. $\psi(u)$ is a characteristic function belonging to the characteristic value λ if

$$\psi(u) = \lambda \int_{-\infty}^\infty \psi(x) e^{2\pi i u x} \, dx \quad \dots (8)$$

There are infinitely many solutions to the integral

equation (8). A particular set of great importance are the *Hermite functions* $\phi_n(\sqrt{2\pi}x)$, which we have already indicated in equation 2.5.1 (10) to be characteristic functions of the operator T with characteristic values (i^n) .

The fundamental mathematical operations as applied to Fourier transforms are listed in Table 2.5.3A, which is modelled on that given by Campbell and Foster; the notation of the tables in this section parallels theirs, $f(x)$ corresponding to $F(f)$ in their listing and $F(u)$ to $G(g)$. In using any tables of Fourier transforms care must be taken to observe the lack of full symmetry between the operations T and T^{-1} . Reference to the tables indicates that in some cases the symmetry is complete, while in others the relation A14 (see Table 2.5.3A) indicates the change which must be made in using a function which appears in the $f(x)$ column as $F(u)$ and vice versa.

In addition to the basic formulae given in Table 2.5.3A, the following results are of importance. These are all special cases of the important *convolution formulae* A8 and A9 given in Table 2.5.3A, and are related to Parseval's equation 2.5.1(6). We have

$$\int_{-\infty}^\infty f(x)g(\pm x) \, dx = \int_{-\infty}^\infty F(u)G(\mp u) \, du \quad \dots (9)$$

$$\int_{-\infty}^\infty f(x)\tilde{g}(x) \, dx = \int_{-\infty}^\infty F(u)\tilde{G}(u) \, du \quad \dots (10)$$

and in particular

$$\int_{-\infty}^\infty |f(x)|^2 \, dx = \int_{-\infty}^\infty |F(u)|^2 \, du \quad \dots (11)$$

Note, however, that $\int f^2(x) \, dx$ is not necessarily equal to $\int F^2(u) \, du$.

In addition to the theoretical importance of the convolution formulae A8 and A9, these results are of central practical importance in many phases of X-ray diffraction theory. Since these results are equally applicable both to Fourier series and to Fourier transforms, a separate section following those on Fourier series is devoted to their discussion (2.5.4.10, page 81).

2.5.3.2. EVALUATION OF FOURIER TRANSFORMS

It is beyond the scope of these tables to discuss the methods which are available for the evaluation of Fourier transforms. Such methods are discussed in detail in the references given in the bibliography.

A brief table of Fourier transforms of special interest to crystallographers is given in Table 2.5.3B, and a list of the most important tabulations is appended.

The Fourier transforms of three special types of functions are of particular importance in crystallography.

TABLE 2.5.3A

Properties of Fourier Transforms

$f(x)$	$F(u)$
1. $f(x) = \int_{-\infty}^{\infty} F(u) e^{-2\pi i u x} du = T^{-1}[F(u)]$	$F(u) = \int_{-\infty}^{\infty} f(x) e^{2\pi i u x} dx = T[f(x)]$
2. $C_1 f_1(x) + C_2 f_2(x)$	$C_1 F_1(u) + C_2 F_2(u)$
3.1. $f(ax)$	$\left. \begin{array}{l} F(u/a)/a \\ F(au) \end{array} \right\} a \text{ is a positive real constant.}$
3.2. $f(x/a)/a$	
4. $f(-x)$	$F(-u)$
5. $f(x) \pm f(-x)$	$F(u) \pm F(-u)$
6.1. $f(x - x_0)$	$e^{2\pi i u x_0} F(u)$
6.2. $e^{-2\pi i u_0 x} f(x)$	$F(u - u_0)$
7. $\tilde{f}(\pm x)$	$\tilde{F}(\mp u)$
†8.1. $f(x)g(x)$	$\int_{-\infty}^{\infty} F(u - \eta) G(\eta) d\eta = \int_{-\infty}^{\infty} F(\eta) G(u - \eta) d\eta$
†8.2. $\int_{-\infty}^{\infty} f(\eta) g(x - \eta) d\eta = \int_{-\infty}^{\infty} f(x - \eta) g(\eta) d\eta$	$F(u)G(u)$
†9.1. $f(x)\tilde{g}(x)$	$\int_{-\infty}^{\infty} F(u + \eta) \tilde{G}(\eta) d\eta = \int_{-\infty}^{\infty} F(\eta) \tilde{G}(\eta - u) d\eta$
†9.2. $\int_{-\infty}^{\infty} f(x + \eta) \tilde{g}(\eta) d\eta = \int_{-\infty}^{\infty} f(\eta) \tilde{g}(\eta - x) d\eta$	$F(u)\tilde{G}(u)$
10.1. df/dx	$-2\pi i u F(u)$
10.2. $2\pi i x f(x)$	dF/du
11. $\partial f(x, \lambda)/\partial \lambda$	$\partial F(u, \lambda)/\partial \lambda$
12.1. $\int_{-\infty}^x f(x) dx$	$-F(u)/2\pi i u$
12.2. $f(x)/2\pi i x$	$\int_{-\infty}^u F(u) du$
13. $\int_{\lambda_0}^{\lambda} f(x, \lambda) d\lambda$	$\int_{\lambda_0}^{\lambda} F(u, \lambda) d\lambda$
14. $F(\pm x)$	$f(\mp u)$

† The formulae given here are typical of the convolution formulae. A discussion of all the possible formulae of this type, derived by successive application of A4 and A7, is given in 2.5.4.10 (page 81).

2.5. FOURIER THEORY

TABLE 2.5.3B
Some Fourier Transforms

$f(x)$	$F(u)$
1.1. $e^{-2\pi i u_0 x}$	$\delta(u - u_0)$
1.2. $\delta(x - x_0)$	$e^{2\pi i u x_0}$
2. $\phi_n\{\sqrt{(2\pi)}x\}$	$i^n \phi_n\{\sqrt{(2\pi)}u\}$ Note A
2.1. $\phi_n(\alpha x)$	$i^n \phi_n(2\pi u/\alpha)$ Note A
2.2. $\frac{1}{\beta} e^{-\pi x^2/\beta^2} \left(\frac{1}{\beta} \int_{-\infty}^{\infty} e^{-\pi x^2/\beta^2} dx = 1 \right)$	$e^{-\pi \beta^2 u^2}$
3. $f(x) = a, x < b$ $= 0, x > b$	$2ab \sin 2\pi ub / 2\pi ub$ Note B
4. $f(x) = a(1 - x/b), x < b$ $= 0, x > b$	$ab(\sin \pi ub / \pi ub)^2$ Note B
5. $f(x) = a(1 - 3x^2/b^2), x < b/3$ $= (3a/2)(1 - 2 x/b + x^2/b^2), b/3 < x < b$ $= 0, x > b$	$(8ab/9)[\sin(2\pi ub/3)/(2\pi ub/3)]^3$ Note B
6. $f(x) = a[1 - 6 x/b ^2 + 6 x/b ^3], x < b/2$ $= 2a(1 - x/b)^3, b/2 < x < b$ $= 0, x > b$	$(3ab/4)[\sin(\pi ub/2)/(\pi ub/2)]^4$ Note B
7. $f(x) = a(1 - x^2/b^2), x < b$ $= 0, x > b$	$(4ab/3) \cdot 3[\sin 2\pi ub - (2\pi ub) \cos 2\pi ub] / (2\pi ub)^3$ Note B
8. $f(x) = a[1 - 3(x/b)^2 + 2 x/b ^3], x < b$ $= 0, x > b$	$ab \frac{\sin \pi ub}{\pi ub} \frac{3[\sin \pi ub - \pi ub \cos \pi ub]}{(\pi ub)^3}$ Note B
9. $f(x) = a[1 - 6(x/b)^2 + 8 x/b ^3 - 3(x/b)^4], x < b$ $= 0, x > b$	$(4ab/5) \cdot 60[2\pi ub(2 + \cos 2\pi ub) - 3 \sin 2\pi ub] / (2\pi ub)^5$ Note B
10. $f(x) = ae^{2\pi i x/\lambda}, x < b$ $= 0, x > b$	$\frac{\lambda a}{\pi} \frac{\sin 2\pi b(u + 1/\lambda)}{(u\lambda + 1)}$ Special cases (p integer): $b = p\lambda; \frac{\lambda a}{\pi} \frac{\sin 2\pi ub}{(u\lambda + 1)}$ $b = (2p + 1)\lambda/2; -\frac{\lambda a}{\pi} \frac{\sin 2\pi ub}{(u\lambda + 1)}$ $b = (4p \pm 1)\lambda/4; \pm \frac{\lambda a}{\pi} \frac{\cos 2\pi ub}{(u\lambda + 1)}$
10.1. $f(x) = a \cos \pi x/2b, x < b$ $= 0, x > b$	$(4ab/\pi) \cos 2\pi ub / (1 - 16u^2b^2)$
11. $ae^{-\alpha x }$	$(2a/\alpha)\alpha^2/(\alpha^2 + 4\pi^2 u^2)$

NOTE A. For the properties of $\phi_n(\alpha x)$ see equations 2.5.1 (8)–(12).

NOTE B. Fourier transforms of the types B 3–9 can be evaluated by the methods of 2.5.3.2(b). See examples 1–3 of that section in connection with the transforms B 4, 7 and 6 respectively.

The Fourier transform of a periodic function is discussed in 2.5.4.2 (page 73). We now discuss the Fourier transforms of "atomic" functions and of functions which can be specified in terms of their discontinuities.

(a) Fourier Transforms of Atomic Functions

By a single "atomic function" we mean a density distribution which has a single maximum and falls monotonically to a negligibly small value on either side of the maximum. Such an atomic distribution may or may not be symmetric. Consider now a function $\rho(x)$ which is built up of a number of such atomic functions $\rho_i(x-a_i)$ with their maxima or arbitrarily specified origins at a_i , i.e.

$$\rho(x) = \sum_{i=1}^n \rho_i(x-a_i) \quad \dots (12)$$

The Fourier transform of such a distribution is then given by

$$F(u) = \sum_{i=1}^n f_i(u) e^{2\pi i u a_i} \quad \dots (13)$$

where $f_i(u)$ is the Fourier transform of $\rho_i(x)$. This result follows directly from A5 and A6.1.

(b) Fourier Transforms of Functions specified by their Discontinuities

Consider a function $f(x)$ which is zero outside a finite range,[†] and which is continuous with continuous derivatives except at a finite number of points α_i at which the function and its derivatives may have discontinuities.

$$\text{If } \Delta f^{(n)}(\alpha_i) = \lim_{\epsilon \rightarrow 0} \{f^{(n)}(\alpha_i + \epsilon) - f^{(n)}(\alpha_i - \epsilon)\} \quad \dots (14)$$

is the discontinuity in the n th derivative $f^{(n)}$ at α_i it can be shown by integrating by parts that

$$F(u) = \sum_{\alpha_i} \left\{ -\frac{\Delta f(\alpha_i)}{2\pi i u} e^{2\pi i u \alpha_i} + \frac{\Delta f^{(1)}(\alpha_i)}{(2\pi i u)^2} e^{2\pi i u \alpha_i} - \frac{\Delta f^{(2)}(\alpha_i)}{(2\pi i u)^3} e^{2\pi i u \alpha_i} + \frac{\Delta f^{(3)}(\alpha_i)}{(2\pi i u)^4} e^{2\pi i u \alpha_i} - \dots \right\} \quad \dots (15)$$

Fourier transforms which can be written in the form (15) are clearly transforms of discontinuous functions, and thus (15) can be used to obtain the discontinuities of $f(x)$ as indicated in the examples.

EXAMPLE 1

$$f(x) = 1 - |x| \quad |x| < 1$$

$$= 0 \quad |x| > 1$$

$$x = -1 \quad \Delta f^{(1)}(-1) = 1$$

$$x = 0 \quad \Delta f^{(1)}(0) = -2 \quad \text{No other discontinuities}$$

$$x = 1 \quad \Delta f^{(1)}(1) = 1$$

$$F(u) = \frac{1}{(2\pi i u)^2} \left\{ e^{-2\pi i u} - 2 + e^{2\pi i u} \right\} = \left(\frac{\sin \pi u}{\pi u} \right)^2$$

EXAMPLE 2

$$f(x) = 1 - x^2 \quad |x| < 1 \quad \frac{dy}{dx} = -2x$$

$$= 0 \quad |x| > 1 \quad \frac{d^2 y}{dx^2} = -2$$

$$x = -1 \quad \Delta f^{(1)} = 2 \quad \Delta f^{(2)} = -2$$

$$x = 1 \quad \Delta f^{(1)} = 2 \quad \Delta f^{(2)} = 2$$

$$F(u) = \frac{2}{(2\pi i u)^2} (e^{-2\pi i u} + e^{2\pi i u}) - \frac{2}{(2\pi i u)^3} (-e^{-2\pi i u} + e^{2\pi i u})$$

$$= \frac{4}{(2\pi u)^3} [\sin 2\pi u - 2\pi u \cos 2\pi u]$$

Note that $\int_{-1}^1 (1-x^2) dx = \frac{4}{3}$ and that

$$\lim_{u \rightarrow 0} \frac{3}{(2\pi u)^3} [\sin 2\pi u - 2\pi u \cos 2\pi u] = 1$$

EXAMPLE 3. Consider $F(u) = (\sin \pi u / \pi u)^4$

$$= \frac{1}{(2\pi i u)^4} [e^{-4\pi i u} - 4e^{-2\pi i u} + 6 - 4e^{2\pi i u} + e^{4\pi i u}]$$

The discontinuities are clearly all in $f^{(3)}$, and since $F(u)$ is real, $f(x)$ must have a centre of symmetry. There are clearly four segments in which $f(x)$ will have different forms, as follows:

$$\begin{array}{ll} -2 < x < -1 & B_0 + B_1 x + B_2 x^2 + B_3 x^3 \\ -1 < x < 0 & A_0 + A_1 x + A_2 x^2 + A_3 x^3 \\ 0 < x < 1 & A_0 - A_1 x + A_2 x^2 - A_3 x^3 \\ 1 < x < 2 & B_0 - B_1 x + B_2 x^2 - B_3 x^3 \end{array}$$

We know from the fact that $f^{(4)} = 0$ at all boundary points that coefficients of x^4 must be zero. It is then not difficult to show that the segments of $f(x)$ are

$$\begin{array}{ll} -2 < x < -1 & f(x) = \frac{1}{6}(2+x)^3 \\ -1 < x < 0 & = \frac{1}{6}[4-6x^2-3x^3] \\ 0 < x < 1 & = \frac{1}{6}[4-6x^2+3x^3] \\ 1 < x < 2 & = \frac{1}{6}(2-x)^3 \end{array}$$

This function may of course be described more briefly as follows:

$$f(x) = 0 \quad |x| > 2$$

$$= \frac{1}{6}(2-|x|)^3 \quad 2 > |x| > 1$$

$$= \frac{1}{6}(4-6x^2+3|x|^3) \quad 1 > |x|$$

This function is the self-convolution of the triangular peak function whose Fourier transform is $(\sin \pi u / \pi u)^2$, which in its turn is the self-convolution of the step function whose Fourier transform is $\sin \pi u / \pi u$.

(c) Fourier Transforms of Empirical Functions

Fourier transforms of empirical functions can be calculated by methods similar to those used for the Fourier analysis of empirical functions (2.5.4.5, page

[†] This condition may be relaxed under special circumstances, but certain precautions must then be taken in applying the method (see [63]).

75). An alternative procedure consists in fitting the empirical function as well as possible in terms of the Hermite functions or other functions whose transforms are known.

2.5.3.3. FOURIER TRANSFORMS IN TWO AND THREE DIMENSIONS

The Fourier transform in three dimensions is expressible in the form

$$f(x_1x_2x_3) = \iiint_{-\infty}^{\infty} F(u_1u_2u_3) e^{-2\pi i(u_1x_1 + u_2x_2 + u_3x_3)} du_1 du_2 du_3 \quad \dots (15a)$$

and its inversion

$$F(u_1u_2u_3) = \iiint_{-\infty}^{\infty} f(x_1x_2x_3) e^{2\pi i(u_1x_1 + u_2x_2 + u_3x_3)} dx_1 dx_2 dx_3 \quad \dots (15b)$$

Such Fourier transforms may usually be evaluated by successive integrations with respect to the individual variables. The many-dimensional Fourier transform operation T forms a group of order 4 as in the one-dimensional case.

Fourier sine and cosine transforms can also be defined in two or more dimensions, but they will not be discussed here.

The mathematical properties of three-dimensional Fourier transforms are in every way analogous to those of the one-dimensional transforms, and every result of Table 2.5.3A can be generalized for three dimensions. In Table 2.5.3C some of the most important and less obvious generalizations of Table 2.5.3A are made explicitly. Others can easily be carried out by the reader.

In our discussion of the Fourier transform we have

set up our definitions in such a manner that the physical dimensions of f and of F shall be the same, that is to say we have chosen the co-ordinates x_1, x_2, x_3 , etc., u_1, u_2, u_3 , etc., to be dimensionless. Thus a displacement vector \mathbf{x} is defined as

$$\mathbf{x} = \sum_i x_i \mathbf{a}_i \quad \dots (16a)$$

where the base vectors \mathbf{a}_i have dimensions of length. Similarly the reciprocal vector \mathbf{u} having the dimensions of reciprocal length is defined as

$$\mathbf{u} = \sum_i u_i \mathbf{a}_i^* \quad \dots (16b)$$

where the reciprocal base vectors \mathbf{a}_i^* have dimensions of reciprocal length.

In the physical problem of most interest to crystallographers the scattering in a direction \mathbf{s} due to a plane parallel beam of wavelength λ in the direction \mathbf{s}_0 is given by

$$F(\mathbf{u}) = \iiint_{-\infty}^{\infty} \rho(\mathbf{x}) e^{2\pi i \mathbf{u} \cdot \mathbf{x}} dV_x = V \iiint_{-\infty}^{\infty} \rho(\mathbf{x}) e^{2\pi i \mathbf{u} \cdot \mathbf{x}} dx_1 dx_2 dx_3 \quad \dots (17a)$$

where $\mathbf{u} = (\mathbf{s} - \mathbf{s}_0)/\lambda$, and dV_x is an element of volume in \mathbf{x} space. This latter is given by $dV_x = V dx_1 dx_2 dx_3$ where V is the volume of an elementary cell of the triplet $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$. Thus $F(\mathbf{u})$ is the Fourier transform of $V\rho(\mathbf{x})$ and conversely

$$\rho(\mathbf{x}) = \frac{1}{V} \iiint_{-\infty}^{\infty} F(\mathbf{u}) e^{-2\pi i \mathbf{u} \cdot \mathbf{x}} du_1 du_2 du_3 = \iiint_{-\infty}^{\infty} F(\mathbf{u}) e^{-2\pi i \mathbf{u} \cdot \mathbf{x}} dV_u \quad \dots (17b)$$

Note that the argument $(\mathbf{u} \cdot \mathbf{x})$ of the kernels $e^{\pm 2\pi i \mathbf{u} \cdot \mathbf{x}}$ must always be dimensionless.

If the triplet \mathbf{a}_i consists of orthogonal unit vectors,

TABLE 2.5.3C

Properties of Three-dimensional Transforms

The numbering corresponds to that of Table 2.5.3A. For the other entries of Table 2.5.3A the generalizations are obvious.

$f(\mathbf{x})$	$F(\mathbf{u})$
1. $f(\mathbf{x}) = \iiint_{-\infty}^{\infty} F(\mathbf{u}) e^{-2\pi i \mathbf{u} \cdot \mathbf{x}} du_1 du_2 du_3$	$F(\mathbf{u}) = \iiint_{-\infty}^{\infty} f(\mathbf{x}) e^{2\pi i \mathbf{u} \cdot \mathbf{x}} dx_1 dx_2 dx_3$
3.1. $f(\alpha \mathbf{x})$	$\left. \begin{array}{l} F(\mathbf{u} \alpha^{-1}) \\ F(\alpha \mathbf{u}) \end{array} \right\} \alpha \text{ is any unitary matrix, i.e. } \alpha = \pm 1.$
3.2. $f(\mathbf{x} \alpha^{-1})$	
10.1. $\partial f(\mathbf{x}) / \partial x_i$	$-2\pi i u_i F(\mathbf{u})$
10.2. $2\pi i x_i f(\mathbf{x})$	$\partial F(\mathbf{u}) / \partial u_i$

2.5. FOURIER THEORY

the Fourier transform can be expressed in cylindrical or in polar co-ordinates as follows:

(a) *Cylindrical Co-ordinates* (see 2.4.3.4, page 53)

If s, ϕ, z are cylindrical co-ordinates in f -space referred to a given plane and zero direction, and S, Φ, Z are corresponding co-ordinates in F -space, (15a) may be written

$$f(s, \phi, z) = \int_0^\infty \int_0^{2\pi} \int_{-\infty}^\infty F(S, \Phi, Z) e^{-2\pi i [sS \cos(\phi - \Phi) + zZ]} S dS d\Phi dZ \quad \dots (18)$$

with an obvious form for the inverse transform (15b). If $f(s, \phi, z)$ is independent of ϕ , (18) becomes

$$f(s, z) = 2\pi \int_0^\infty \int_{-\infty}^\infty F(S, Z) J_0(2\pi sS) e^{-2\pi i zZ} S dS dZ \quad \dots (18a)$$

with a similar expression for the inverse transform. In (18a) and (18b) below, $J_0(2\pi sS)$ is the zero order

Bessel function (see [1]). If $f(s, \phi, z)$ depends only on s , (18) takes the form

$$f(s) = 2\pi \int_0^\infty F(S) J_0(2\pi sS) S dS \quad \dots (18b)$$

with an analogous inverse. Note that in this case the three-dimensional transform is given by

$$F(S, \Phi, Z) = F(S) \delta(Z) \quad \dots (18b')$$

where $\delta(Z)$ is the delta function.

(b) *Polar Co-ordinates* (see 2.4.3.4, page 53)

If r, θ, ϕ are polar co-ordinates in f -space referred to a given pole and zero meridian, and R, Θ, Φ are corresponding co-ordinates in F -space, then (15a) becomes

$$f(r, \theta, \phi) = \int_0^\infty \int_0^\pi \int_0^{2\pi} F(R, \Theta, \Phi) e^{-2\pi i rR [\cos \theta \cos \Theta + \sin \theta \sin \Theta \cos(\phi - \Phi)]} R^2 \sin \Theta dR d\Theta d\Phi \quad \dots (19)$$

TABLE 2.5.3D

Some Three-dimensional Fourier Transforms

$$\begin{aligned} \text{Notation: } s^2 &= x_2^2/b_2^2 + x_3^2/b_3^2 \\ r^2 &= x_1^2/b_1^2 + x_2^2/b_2^2 + x_3^2/b_3^2 \end{aligned}$$

$$\begin{aligned} S^2 &= u_2^2/b_2^2 + u_3^2/b_3^2 \\ R^2 &= u_1^2/b_1^2 + u_2^2/b_2^2 + u_3^2/b_3^2 \end{aligned}$$

$f(x)$	$F(u)$
1.1. $e^{-2\pi i u_0 \cdot x}$	$\delta(u - u_0)$
1.2. $\delta(x - x_0)$	$e^{2\pi i u \cdot x_0}$
2. $\phi_m\{\sqrt{(2\pi)}x_1\} \phi_n\{\sqrt{(2\pi)}x_2\} \phi_p\{\sqrt{(2\pi)}x_3\}$	$i^{m+n+p} \phi_m\{\sqrt{(2\pi)}u_1\} \phi_n\{\sqrt{(2\pi)}u_2\} \phi_p\{\sqrt{(2\pi)}u_3\}$
2.1. $\phi_m(\alpha_1 x_1) \phi_n(\alpha_2 x_2) \phi_p(\alpha_3 x_3)$	$i^{m+n+p} \phi_m(2\pi u_1/\alpha_1) \phi_n(2\pi u_2/\alpha_2) \phi_p(2\pi u_3/\alpha_3)$
2.2. $\frac{1}{b_1 b_2 b_3} e^{-\pi r^2}$	$e^{-\pi R^2}$
3.1. $f(x) = a, x_i < b_i$ $= 0, x_i > b_i$	$(8ab_1 b_2 b_3) \frac{\sin 2\pi u_1 b_1}{2\pi u_1 b_1} \frac{\sin 2\pi u_2 b_2}{2\pi u_2 b_2} \frac{\sin 2\pi u_3 b_3}{2\pi u_3 b_3}$
3.2. $f(x) = a, x_1 < b_1$ and $s^2 < 1$ $= 0, x_1 > b_1$ or $s^2 > 1$	$(4\pi a b_1 b_2 b_3) \frac{\sin 2\pi u_1 b_1}{2\pi u_1 b_1} \frac{J_1(2\pi S)}{(2\pi S)}$
3.3. $f(x) = a$ $r^2 < 1$ $= 0$ $r^2 > 1$	$\left(\frac{4}{3}\pi a b_1 b_2 b_3\right) \frac{3(\sin 2\pi R - 2\pi R \cos 2\pi R)}{(2\pi R)^3}$
4. $f(x) = a(1 - r)$ $r^2 < 1$ $= 0$ $r^2 > 1$	$\left(\frac{\pi a}{3} b_1 b_2 b_3\right) \frac{12}{(2\pi R)^4} [2(1 - \cos 2\pi R) - 2\pi R \sin 2\pi R]$
5. $f(x) = a(1 - r^2)$ $r^2 < 1$ $= 0$ $r^2 > 1$	$(8\pi a b_1 b_2 b_3/15) \frac{15}{(2\pi R)^5} \{[3 - (2\pi R)^2] \sin 2\pi R - 3(2\pi R) \cos 2\pi R\}$

with an obvious form for the inverse transform. If $f(r, \theta, \phi)$ is independent of ϕ , (19) becomes

$$f(r, \theta) = 2\pi \int_0^\infty \int_0^\pi F(R, \Theta) J_0(2\pi r R \sin \theta \sin \Theta) e^{-2\pi i r R \cos \theta \cos \Theta} R^2 \sin \Theta dR d\Theta \quad \dots (19a)$$

with an obvious inverse transformation from (15b). If $f(r, \theta, \phi)$ depends only on r , then the transform becomes

$$f(r) = 4\pi \int_0^\infty F(R) \frac{\sin 2\pi r R}{2\pi r R} R^2 dR \quad \dots (19b)$$

with the obvious inverse transformation.

2.5.3.4. EVALUATION OF THREE-DIMENSIONAL FOURIER TRANSFORMS

The evaluation of Fourier transforms in two or three dimensions is usually carried out by successive evaluation of one-dimensional transforms. Fourier transforms for "atomic functions" have exactly the same properties as the one-dimensional transforms, and the details of the generalization need not be given here.

No account seems to be available of a generalization of the method of discontinuities to several dimensions. However, von Laue (*Ann. der Phys.*, **26**, 55, 1936) made use of Gauss's theorem to transform the volume Fourier integral into a surface integral for those cases in which the function $f(x)$ is a constant within a closed surface and zero outside it. Reference must be made to the original paper for a discussion of this method.

A detailed discussion of the relationship between three-, two- and one-dimensional transforms has been given by Waser and Schomaker [66] in a paper which includes a treatment of the relationship between integral and series transforms and many applications of Fourier transform theory to diffraction problems.

Some examples of three-dimensional Fourier transforms are given in Table 2.5.3D, and reference is made to further examples in [61], where some transforms are used as shape functions. See also Section 6.3 for some crystallographic applications of Fourier transforms.

2.5.4. Fourier Series

2.5.4.1. BASIC THEORY

If $f(x)$ is a periodic function of period unity, we write the *Fourier series*

$$f(x) = \sum_{h=-\infty}^{\infty} F(h) e^{-2\pi i h x} \quad \dots (1a)$$

with h integral; and the *Fourier coefficients* are

$$F(h) \equiv \int_0^1 f(x) e^{2\pi i h x} dx \quad \dots (1b)$$

The functions $e^{2\pi i h x}$ in which h takes all positive and negative integral values form a complete orthonormal

set of functions for the periodically repeated range $0 < x < 1$.

If in (1) we separate $F(h)$ into its real and imaginary parts, i.e.

$$F(h) = A(h) + iB(h) \quad \dots (2a)$$

and if $f(x)$ is a real function

$$\left. \begin{aligned} A(h) &= A(\bar{h}) \\ B(h) &= -B(\bar{h}) \end{aligned} \right\} \quad \dots (2b)$$

then the results (1) can be rewritten

$$f(x) = A(0) + 2 \sum_{h=1}^{\infty} A(h) \cos 2\pi h x + 2 \sum_{h=1}^{\infty} B(h) \sin 2\pi h x \quad \dots (3a)$$

$$\text{with } A(0) = \int_0^1 f(x) dx; \quad A(h) = \int_0^1 f(x) \cos 2\pi h x dx$$

$$B(h) = \int_0^1 f(x) \sin 2\pi h x dx \quad \dots (3b)$$

From the general theory of orthogonal functions we have a number of important results. Bessel's formula for a partial sum takes the form

$$\int_0^1 |f(x) - \sum_{h=n}^{n'} F(h) e^{-2\pi i h x}|^2 dx = \int_0^1 |f(x)|^2 dx - \sum_{h=n}^{n'} |F(h)|^2 \quad \dots (4)$$

and the partial sum is the closest possible mean square approximation with the terms used. We also have Bessel's inequality

$$\sum_{h=n}^{n'} |F(h)|^2 < \int_0^1 |f(x)|^2 dx \quad \dots (5)$$

The equality in (5) (Parseval's equation) holds only for the complete set of Fourier coefficients.

In Table 2.5.4A are listed the effects on the Fourier coefficients of the application of certain mathematical operations to $f(x)$. Note the analogy between these results and those for Fourier transforms. Note too that there is even less reason to say that the relation between the periodic function and its coefficients is symmetrical than there is in the case of the more general function and its Fourier transform.

2.5.4.2. FOURIER TRANSFORM OF A PERIODIC FUNCTION

Consider the Fourier transform $\mathcal{F}(u)$ of

$$f(x) = \sum_{h=-\infty}^{\infty} F(h) e^{-2\pi i h x} \quad \dots (6)$$

Since $\int_{-\infty}^{\infty} |f(x)|^2 dx$ is infinite, we have first to consider the transform of the function $f(x) e^{-\pi \alpha^2 x^2}$. We now write

$$\mathcal{F}(u) = \lim_{\alpha \rightarrow 0} \int_{-\infty}^{\infty} \sum_{h=-\infty}^{\infty} F(h) e^{-2\pi i h x} e^{-\pi \alpha^2 x^2} e^{2\pi i u x} dx \quad \dots (7)$$

TABLE 2.5.4A

Properties of Fourier Series

NOTE. (a) $f(x)$ is a real function. (b) The numbers correspond to those of Table 2.5.3A.

$f(x)$	$F(h)$
1. $f(x) = \sum_{h=-\infty}^{\infty} F(h)e^{-2\pi i h x}$	$F(h) = \int_0^1 f(x)e^{2\pi i h x} dx$
2. $C_1 f_1(x) \pm C_2 f_2(x)$	$C_1 F_1(h) \pm C_2 F_2(h)$
4. $f(-x)$	$F(-h)$
5. $f(x) \pm f(-x)$	$F(h) \pm F(-h)$
6.1. $f(x-x_0)$	$e^{2\pi i h x_0} F(h)$
8.1. $f(x)g(x)$	$\sum_{k=-\infty}^{\infty} F(k)G(h-k)$
8.2. $\int_0^1 f(\eta)g(x-\eta)d\eta$	$F(h)G(h)$
9.2. $\int_0^1 f(\eta)g(x+\eta)d\eta$	$\tilde{F}(h)G(h)$
10.1. df/dx	$-2\pi i h F(h)$

Now the integral

$$I(u, \alpha) = \int_{-\infty}^{\infty} e^{-\pi \alpha^2 x^2 + 2\pi i (u-h)x} dx$$

can be rewritten in the form

$$I(u, \alpha) = e^{\frac{-\pi(u-h)^2}{\alpha^2}} \int_{-\infty}^{\infty} e^{-\pi \alpha^2 \left[x - \frac{i(u-h)}{\alpha^2}\right]^2} dx = \frac{1}{\alpha} e^{\frac{-\pi(u-h)^2}{\alpha^2}} \quad \dots (8)$$

Now by 2.5.2 (2) (page 66):

$$\lim_{\alpha \rightarrow 0} I(u, \alpha) = \delta(u-h)$$

and (7) becomes

$$\mathcal{F}(u) = \sum_{h=-\infty}^{\infty} F(h)\delta(u-h) \quad \dots (9)$$

which is zero everywhere except at the whole numbered points $u=h$; and at each such point there is a delta function of weight $F(h)$ (which may, of course, be complex).

2.5.4.3. FOURIER SERIES FOR AN ARBITRARY PERIOD

If the period of a Fourier series is not unity, but is a an arbitrary positive number, there are two pro-

cedures which may be adopted. If we let x be a fraction of the vector period a , such that a vector distance r along the axis is given by

$$r = xa \quad \dots (10)$$

the Fourier series will retain the form (1a) and the coefficients the form (1b). In the case of the Fourier transform $\mathcal{F}(u)$, the vector u is given by 2.5.3 (17) in the form

$$u = ua^* \quad \dots (11)$$

in which $a \cdot a^* = 1$. That is to say, the delta function of weight $F(h)$ will be located at the points ha^* (i.e. h/a).

In the second approach the distance r along the axis is used directly as a variable and the Fourier series (1a) takes the form

$$f(r) = \sum_{h=-\infty}^{\infty} F(h)e^{-2\pi i hr/a} \quad \dots (12a)$$

while the Fourier coefficients are of the form

$$F(h) = \frac{1}{a} \int_0^a f(r)e^{2\pi i hr/a} dr \quad \dots (12b)$$

In this case the Fourier transform with respect to r as a variable will be a set of delta functions at $u=h/a$.

The first approach is the most usual in crystallography and is in general to be recommended. The second approach is of importance when the period must be kept in mind.

2.5.4.4. CALCULATION OF FOURIER COEFFICIENTS

(a) Fourier Series for the Periodic Repetition of an Arbitrary Function

Let $\phi_0(x)$ be an arbitrary function with Fourier transform $\Phi_0(u)$, the variables x and u being scaled in terms of unit vectors reciprocal to one another. Now consider the periodic function

$$\phi(x) = \sum_{n=-\infty}^{\infty} \phi_0(x-na) = \sum_{h=-\infty}^{\infty} \Phi(h) e^{-2\pi i h x/a} \dots (13a)$$

Then

$$\begin{aligned} \Phi(h) &= \frac{1}{a} \int_{-\infty}^{\infty} \phi_0(x-na) e^{2\pi i h x/a} dx = \frac{1}{a} \int_{-\infty}^{\infty} \phi_0(x) e^{2\pi i h x/a} dx \\ &= \frac{1}{a} \Phi_0(h/a) \dots (13b) \end{aligned}$$

and the Fourier coefficients are simply the sampling of the Fourier transform at the points $u=h/a$ with the appropriate scale factor $1/a$. Note that there is no restriction as to the non-zero range of $\phi_0(x)$ in this result: it may be entirely confined to the period or extend over the infinite range.

The way in which this result is to be applied to the calculation of the Fourier coefficients of a set of atomic functions, i.e. of a set of structure factors, is discussed more clearly in terms of the three-dimensional series in 2.5.4.9 (page 80).

(b) The Fourier Series of a Function determined by its Discontinuities

The result for the Fourier series of period unity is identical with that for the Fourier transform as given in 2.5.3 (15):

$$\begin{aligned} F(h) &= \sum_{\alpha_i} \left\{ -\frac{\Delta f(\alpha_i)}{2\pi i h} e^{2\pi i h \alpha_i} + \frac{\Delta f^{(1)}(\alpha_i)}{(2\pi i h)^2} e^{2\pi i h \alpha_i} \right. \\ &\quad \left. - \frac{\Delta f^{(2)}(\alpha_i)}{(2\pi i h)^3} e^{2\pi i h \alpha_i} + \frac{\Delta f^{(3)}(\alpha_i)}{(2\pi i h)^4} e^{2\pi i h \alpha_i} - \dots \right\} \dots (14) \end{aligned}$$

except that the co-ordinates of the discontinuities can now be limited to the range $0 < \alpha_i < 1$, and h is integral.

(c) Tabulations of Fourier Coefficients for Various Functions

Table 2.5.4B gives a brief list of the Fourier coefficients for a few functions which may be of importance in crystal structure calculations. This list may be amplified by the use of (13) and Table 2.5.3B or any other table of Fourier transforms. Tables of Fourier series coefficients are also available in [63].

2.5.4.5. NUMERICAL CALCULATIONS FOR FOURIER SERIES

(a) Summation at N Equidistant Points

The Fourier series $f(x)$ of period a is to be summed at the N equidistant points ra/N , where N is an integer assumed to be divisible by 4.† The Fourier series then takes the form

$$\begin{aligned} f(ra/N) &= \sum_{h=-\infty}^{\infty} F(h) e^{-2\pi i h r/N} \\ &= c_e(ra/N) + c_o(ra/N) + s_e(ra/N) + s_o(ra/N) \dots (15) \end{aligned}$$

The four sums are

$$\begin{aligned} c_e(ra/N) &= \sum_{p=0}^{N/4} C(2p) \cos 2\pi 2pr/N \\ c_o(ra/N) &= \sum_{p=0}^{N/4-1} C(2p+1) \cos 2\pi (2p+1)r/N \\ s_e(ra/N) &= \sum_{p=1}^{N/4-1} S(2p) \sin 2\pi 2pr/N \\ s_o(ra/N) &= \sum_{p=0}^{N/4-1} S(2p+1) \sin 2\pi (2p+1)r/N \end{aligned} \dots (16)$$

In these sums the coefficients $C(h)$ and $S(h)$ are related to the Fourier coefficients $F(h) = A(h) + iB(h)$ by the expressions

$$\begin{aligned} C(h) &= \sum_{s=-\infty}^{\infty} [A(sN+h) + A(sN-h)] \\ S(h) &= \sum_{s=-\infty}^{\infty} [B(sN+h) - B(sN-h)] \\ C(0) &= \sum_{s=-\infty}^{\infty} A(sN) \\ C\left(\frac{N}{2}\right) &= \sum_{s=-\infty}^{\infty} A[(2s+1)N/2] \end{aligned} \dots (17)$$

If, as is usually the case, the Fourier coefficients $F(h)$ are negligibly small for $h > N/2$ and $f(x)$ is real, the expressions (17) take the simpler forms:

$$\begin{aligned} C(h) &= 2A(h); \quad C(0) = A(0); \quad C(N/2) = 2A(N/2); \\ S(h) &= 2B(h) \dots (18) \end{aligned}$$

Note that the sine coefficients $B(sN/2)$ make no contribution to the series at the points ra/N .

It is only necessary to calculate the sums (16) for the range $0 \leq r \leq N/4$, since we have

$$\begin{aligned} f(ra/N) &= c_e + c_o + s_e + s_o \\ f\left[\left(\frac{N}{2} - r\right)a/N\right] &= c_e - c_o - s_e + s_o \\ f\left[\left(\frac{N}{2} + r\right)a/N\right] &= c_e - c_o + s_e - s_o \\ f[(N-r)a/N] &= c_e + c_o - s_e - s_o \end{aligned} \dots (19)$$

† This assumption is required by the usual strip methods of Fourier summation. For schemes using other values of N see [42].

TABLE 2.5.4B
Some Fourier Series

	$f(x)$	$F(0)$	$F(h)$	$A(h)$	$B(h)$
1.1	$=a; x < \alpha$ $=0; \text{elsewhere}$	$2\alpha a$	$2\alpha a \sin 2\pi h\alpha/2\pi h\alpha$	$F(h)$	0
1.2	$=a; -\frac{1}{4} < x < \frac{1}{4}$ $=-a; \frac{1}{4} < x < \frac{3}{4}$	0	$(-1)^n 2a/\pi h; h=2n+1$ 0; $h=2n$	$F(h)$	0
1.3	$=a; 0 < x < \frac{1}{2}$ $=-a; \frac{1}{2} < x < 1$	0	$2ia/\pi h; h=2n+1$ 0; $h=2n$	0	$-iF(h)$
2.1	$=a(1+x/\alpha_1); -\alpha_1 < x < 0$ $=a(1-x/\alpha_2); 0 < x < \alpha_2$ $=0; \text{elsewhere}$	$a(\alpha_1 + \alpha_2)/2$	$\frac{ia}{2\pi h} \left\{ e^{-\pi i h \alpha_1} \frac{\sin \pi h \alpha_1}{\pi h \alpha_1} - e^{\pi i h \alpha_2} \frac{\sin \pi h \alpha_2}{\pi h \alpha_2} \right\}$	$\frac{a}{2\pi h} \left\{ \frac{\sin^2 \pi h \alpha_1}{\pi h \alpha_1} + \frac{\sin^2 \pi h \alpha_2}{\pi h \alpha_2} \right\}$	$\frac{a}{2\pi h} \left\{ \frac{\sin 2\pi h \alpha_1}{2\pi h \alpha_1} - \frac{\sin 2\pi h \alpha_2}{2\pi h \alpha_2} \right\}$
2.2	$=a(1+x/\alpha); -\alpha < x < 0$ $=a(1-x/\alpha); 0 < x < \alpha$ $=0; \text{elsewhere}$	$a\alpha$	$a\alpha(\sin \pi h\alpha/\pi h\alpha)^2$	$F(h)$	0
2.3	$=ax/\alpha; -\alpha < x < \alpha$ $=a(1-2x)/(1-2\alpha);$ $\alpha < x < 1-\alpha$	0	$ia \sin 2\pi h\alpha/2\pi^2 h^2 \alpha(1-2\alpha)$	0	$-iF(h)$
2.4	$=4ax; -\frac{1}{4} < x < \frac{1}{4}$ $=2a(1-2x); \frac{1}{4} < x < \frac{3}{4}$	0	0; $h=2n$ $4i(-1)^n a/\pi^2 h^2; h=2n+1$	0	$-iF(h)$
2.5	$=a(1+4x); -\frac{1}{2} < x < 0$ $=a(1-4x); 0 < x < \frac{1}{2}$	0	0; $h=2n$ $4a/\pi^2 h^2; h=2n+1$	$F(h)$	0

TABLE 2.5.4B (continued)

	$f(x)$	$F(0)$	$F(h)$	$A(h)$	$B(h)$
3	$=a(1-2x); 0 < x < 1$	0	$ia/\pi h$	0	$-iF(h)$
4.1	$=a(1-x^2/\alpha^2); x < \alpha$ $=0; \text{elsewhere}$	$4a\alpha/3$	$4a\alpha[\sin 2\pi h\alpha - 2\pi h\alpha \cos 2\pi h\alpha]/(2\pi h\alpha)^3$	$F(h)$	0
4.2	$=a(1-16x^2); -\frac{1}{4} < x < \frac{1}{4}$ $=a(3-4x)(1-4x); \frac{1}{4} < x < \frac{3}{4}$	0	0; $h=2n$ $16a(-1)^n/\pi^3 h^3; h=2n+1$	$F(h)$	0
5	$=a(1-16x^2)(5-16x^2)/5;$ $-\frac{1}{4} < x < \frac{1}{4}$ $=-a(1-16\xi^2)(5-16\xi^2)/5;$ $\frac{1}{4} < x < \frac{3}{4}$ $\xi = x - \frac{1}{2}$	0	0; $h=2n$ $(-1)^n 768a/5\pi^5 h^5; h=2n+1$	$F(h)$	0
6.1	$=\cos 2\pi x - \cos 2\pi\alpha;$ $-\alpha < x < \alpha$ $=0; \text{elsewhere}$	$(\sin 2\pi\alpha - 2\pi\alpha \cos 2\pi\alpha)/\pi$	$F(h) = \left\{ \frac{\sin 2\pi h\alpha \cos 2\pi\alpha}{\pi h(h^2-1)} - \frac{\cos 2\pi h\alpha \sin 2\pi\alpha}{\pi(h^2-1)} \right\}$	$F(h)$	0
6.2	$=\cos 2\pi x; -\frac{1}{4} < x < \frac{1}{4}$ $=0; \text{elsewhere}$	$1/\pi$	$F(\pm 1) = \alpha \left\{ 1 - \frac{\sin 4\pi\alpha}{4\pi\alpha} \right\}$ $F(2n+1) = 0; n \neq 0$ $F(\pm 1) = 1/4$ $F(2n) = (-1)^{n+1}/\pi(4n^2-1)$	$F(h)$	0
7	$=ae^{-2\pi\beta x }$	$a/\pi\beta$	$a\beta/\pi(\beta^2+h^2)$	$F(h)$	0
8	$=ae^{-\pi x^2/\beta^2}$	$a\beta$	$a\beta e^{-\pi\beta^2 h^2}$	$F(h)$	0

The principles indicated here are directly applicable to the summation of two- and three-dimensional series. For details see 2.5.4.7.

(b) *Calculation of Coefficients for a Periodic Function known at N Points*

If the function $f(x)$ of period a is known at the N equidistant points $x=ra/N$, the coefficients $C(h)$ and $S(h)$ defined by (17) and (18) can be directly calculated from the relations

$$\left. \begin{aligned} NC(h) &= C_e(h) + C_o(h) \\ NS(h) &= S_e(h) + S_o(h) \end{aligned} \right\} \dots (20)$$

The four sums are analogous to (16) and are

$$\left. \begin{aligned} C_e(h) &= \sum_{q=0}^{N/4} c(2q) \cos 2\pi 2qh/N \\ C_o(h) &= \sum_{q=0}^{N/4-1} c(2q+1) \cos 2\pi(2q+1)h/N \\ S_e(h) &= \sum_{q=1}^{N/4-1} s(2q) \sin 2\pi 2qh/N \\ S_o(h) &= \sum_{q=0}^{N/4-1} s(2q+1) \sin 2\pi(2q+1)h/N \end{aligned} \right\} \dots (21)$$

In these sums the coefficients $c(r)$ and $s(r)$ are given by

$$\left. \begin{aligned} c(r) &= f(ra/N) + f(-ra/N) \\ s(r) &= f(ra/N) - f(-ra/N) \end{aligned} \right\} \dots (22)$$

Again we need only calculate the sums (21) for the range $0 \leq h \leq N/4$, since we have

$$\left. \begin{aligned} NC\left(\frac{N}{2}-h\right) &= C_e(h) - C_o(h) \\ NS\left(\frac{N}{2}-h\right) &= -S_e(h) + S_o(h) \end{aligned} \right\} \dots (23)$$

Equations (18) tell us that $C(h)$ and $S(h)$ determine the Fourier coefficients for $0 \leq h \leq N/2$ (with the exception of $B(N/2)$) if the coefficients outside this range are negligible. Otherwise equations (17) establish relationships between the Fourier coefficients (other than $B(sN/2)$) through the quantities $C(h)$ and $S(h)$.

2.5.4.6. *FOURIER SERIES IN TWO DIMENSIONS*

The function

$$f(x, y) = \sum_{h, k=-\infty}^{\infty} F(hk) e^{-2\pi i(hx+ky)} \dots (24a)$$

is the most general form for the Fourier series in two dimensions. Here

$$F(hk) = \int_0^1 \int_0^1 f(x, y) e^{2\pi i(hx+ky)} dx dy \dots (24b)$$

The Fourier coefficients are in general complex and may be written

$$F(hk) = A(hk) + iB(hk) \dots (25)$$

If $f(x, y)$ is real we have

$$F(hk) = \bar{F}(\bar{h}\bar{k}) \dots (26)$$

$$\text{i.e. } A(hk) = A(\bar{h}\bar{k}); \text{ and } B(hk) = -B(\bar{h}\bar{k}) \dots (27)$$

The series (24a) can be written in the form

$$f(x, y) = \sum_{h, k=-\infty}^{\infty} [A(hk) \cos 2\pi(hx+ky) + B(hk) \sin 2\pi(hx+ky)] \dots (28)$$

In almost all cases two-dimensional Fourier series are handled in terms of the component one-dimensional series. The application of Fourier transforms to the determination of the coefficients of a many-dimensional series will be illustrated in 2.5.4.9 (page 80) in terms of the three-dimensional series.

2.5.4.7. *EXPANSION OF TWO-DIMENSIONAL SERIES IN TERMS OF ONE-DIMENSIONAL SERIES*

Following the suggestion of Beevers and Lipson, the series (28) can be further expanded as follows:

$$\begin{aligned} f(x, y) &= \sum_{h, k=0}^{\infty} CC(hk) \cos 2\pi hx \cos 2\pi ky + \\ &\quad \sum_{h, k=1}^{\infty} SS(hk) \sin 2\pi hx \sin 2\pi ky + \\ &\quad \sum_{h=0}^{\infty} \sum_{k=1}^{\infty} CS(hk) \cos 2\pi hx \sin 2\pi ky + \\ &\quad \sum_{h=1}^{\infty} \sum_{k=0}^{\infty} SC(hk) \sin 2\pi hx \cos 2\pi ky \dots (29) \end{aligned}$$

In this series the summations have been changed from the doubly infinite range to the singly infinite range, and the multiplicities are taken care of by the following expressions:

$$\begin{aligned} CC(hk) &= +A(hk) + A(\bar{h}\bar{k}) + A(\bar{h}k) + A(h\bar{k}) \\ &= 2[+A(hk) + A(\bar{h}\bar{k})] \\ SS(hk) &= -A(hk) - A(\bar{h}\bar{k}) + A(\bar{h}k) + A(h\bar{k}) \\ &= 2[-A(hk) + A(\bar{h}\bar{k})] \\ CS(hk) &= +B(hk) - B(\bar{h}\bar{k}) + B(\bar{h}k) - B(h\bar{k}) \\ &= 2[+B(hk) + B(\bar{h}\bar{k})] \\ SC(hk) &= +B(hk) - B(\bar{h}\bar{k}) - B(\bar{h}k) + B(h\bar{k}) \\ &= 2[+B(hk) + B(\bar{h}\bar{k})] \end{aligned}$$

$$\begin{aligned} CC(0k) &= 2A(0k) & CC(h0) &= 2A(h0) \\ SS(0k) &= 0 & SS(h0) &= 0 \\ CS(0k) &= 2B(0k) & CS(h0) &= 0 \\ SC(0k) &= 0 & SC(h0) &= 2B(h0) \\ CC(00) &= A(00) & SS(00) &= CS(00) = SC(00) = 0 \end{aligned} \dots (30)$$

If the practice of separating odd and even terms is followed, each of the four sums of (29) will lead to four separate sums of different parity which are then combined with different signs to give function values for the sixteen cell "quadrants" by rules which derive from (19). It is usual, however, to do the expansion

2.5. FOURIER THEORY

in two parts. If, for example, summation with respect to h is carried out first, we shall have

$$f(x, y) = \sum_{k=0}^{\infty} C(x, k) \cos 2\pi ky + \sum_{k=1}^{\infty} S(x, k) \sin 2\pi ky \quad \dots (31)$$

in which

$$\begin{aligned} C(x, k) &= \sum_{h=0}^{\infty} CC(hk) \cos 2\pi hx + \sum_{h=1}^{\infty} SC(hk) \sin 2\pi hx \\ &= c_e C(x, k) + c_o C(x, k) + s_e C(x, k) + s_o C(x, k) \end{aligned} \quad \dots (32a)$$

and

$$\begin{aligned} S(x, k) &= \sum_{h=1}^{\infty} SS(hk) \sin 2\pi hx + \sum_{h=0}^{\infty} CS(hk) \cos 2\pi hx \\ &= s_e S(x, k) + s_o S(x, k) + c_e S(x, k) + c_o S(x, k) \end{aligned} \quad \dots (32b)$$

The expansion in range of x is then carried out by rules analogous to (19) before the summation (31) with respect to k is carried out. The rules for expansion are

$$\left. \begin{aligned} C(x, k) &= c_e C + c_o C + s_e C + s_o C \\ C(\tfrac{1}{2}-x, k) &= c_e C - c_o C - s_e C + s_o C \\ C(\tfrac{1}{2}+x, k) &= c_e C - c_o C + s_e C - s_o C \\ C(1-x, k) &= c_e C + c_o C - s_e C - s_o C \end{aligned} \right\} \quad \dots (33a)$$

and also

$$\left. \begin{aligned} S(x, k) &= c_e S + c_o S + s_e S + s_o S \\ S(\tfrac{1}{2}-x, k) &= c_e S - c_o S - s_e S + s_o S \\ S(\tfrac{1}{2}+x, k) &= c_e S - c_o S + s_e S - s_o S \\ S(1-x, k) &= c_e S + c_o S - s_e S - s_o S \end{aligned} \right\} \quad \dots (33b)$$

After the summation (31) over k is completed, the expansion over the necessary range of y values is completed by an identical procedure.

2.5.4.8. SYMMETRY OF THE BEEVERS-LIPSON EXPANSION

There are in all sixteen different summations involved in the complete expansion of a two-dimensional series outlined in 2.5.4.7, and it is only in the case of symmetry $p1$ that all these terms are required. The sum $CC(ee)$ possesses all possible centres, planes, and glide planes which can occur in any possible setting of any plane group of the plane point groups 1, 2, m , $2mm$. In addition this sum possesses all the possible half-translations (i.e. $\frac{1}{2}0$, $0\frac{1}{2}$, $\frac{1}{2}\frac{1}{2}$). The sum $CC(ee)$ occurs in all Fourier series. In each of the other fifteen sums, half of the symmetry elements are replaced by antisymmetry elements (cf. Cochran, *Acta*, 5, 630, 1952), and the combination of one such term with $CC(ee)$ will remove those elements from $CC(ee)$ which correspond to the antisymmetry elements in the added term. Table 2.5.4C lists the symmetry and antisymmetry elements of each of the sixteen types of terms in the Beevers-Lipson summation. The application of this permits a rapid decision as to the terms which will appear in the summation for any given plane group, in

that no term can appear which possesses an antisymmetry element to correspond to a symmetry element in the plane group of the summation. The process of elimination is best illustrated by examples.

EXAMPLE 1

Plane group $p2mg$ with axes at $\frac{1}{4}\frac{1}{4}$. The symmetry elements are then: 2 at $\frac{1}{4}\frac{1}{4}$; m in $0v$; g in $u\frac{1}{4}$. The elimination is then indicated by the square array

	CC	CS	SC	SS
ee		2g	2m	gm
eo	2g		gm	2m
oe	2g		gm	2m
oo		2g	2m	gm

Remaining terms: $CC(ee)(oo)$; $CS(eo)(oe)$.

EXAMPLE 2

Plane group $clm1$. The symmetry elements are: c ; m in $0v$; g in $\frac{1}{4}v$; and the elimination table reads

		gm	gm
cg	cg	cm	cm
cg	cg	cm	cm
		gm	gm

Remaining terms: $CC(ee)(oo)$; $CS(ee)(oo)$.

It should be noticed that there is no inherent advantage to the location of the twofold axis at the origin in computing a two-dimensional series. The presence of the axis decides the number of terms which have to be computed whether or not the axis is at the origin.

Symmetry operations of the plane group other than those listed in Table 2.5.4C do not affect the number of terms in the summation, but they may reduce the area of the region for which the function need be calculated as do the operations of Table 2.5.4C. In such plane groups one can only make use of the symmetry of the classes 2, m and $2mm$. This process is illustrated by an example.

EXAMPLE 3

Plane group $p6mm$ referred to hexagonal axes with 6 at 00. If the Fourier series in this plane group is calculated in terms of the hexagonal axes, the only effective symmetry element will be the 2 axis at 00 and the series will contain all the terms CC and all the terms SS . Calculation of one quarter-cell will not exhibit the full asymmetric unit of $p6mm$. However, calculation of the half-cell, which is logical for $p2$, will exhibit the asymmetric unit of $p6mm$ six times.

2.5. FOURIER THEORY

TABLE 2.5.4C

Symmetry and Antisymmetry Properties of Beavers-Lipson Summation

+ indicates symmetry element
 - indicates antisymmetry element

		Translations 1				Axes 2				Mirror Planes <i>m</i>				Glide Planes <i>g</i>			
		00	$\frac{1}{2}0$	$0\frac{1}{2}$	$\frac{1}{2}\frac{1}{2}$	00	$\frac{1}{2}0$	$0\frac{1}{2}$	$\frac{1}{2}\frac{1}{2}$	0 <i>v</i>	$\frac{1}{4}v$	<i>u</i> 0	$u\frac{1}{4}$	0 <i>v</i>	$\frac{1}{4}v$	<i>u</i> 0	$u\frac{1}{4}$
CC	ee	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+
	eo	+	+	-	-	+	+	-	-	+	+	+	-	-	-	+	-
	oe	+	-	+	-	+	-	+	-	+	-	+	+	+	-	-	-
	oo	+	-	-	+	+	-	-	+	+	-	+	-	-	+	-	+
CS	ee	+	+	+	+	-	-	-	-	+	+	-	-	+	+	-	-
	eo	+	+	-	-	-	-	+	+	+	+	-	+	-	-	-	+
	oe	+	-	+	-	-	+	-	+	+	-	-	-	+	-	+	+
	oo	+	-	-	+	-	+	+	-	+	-	-	+	-	+	+	-
SC	ee	+	+	+	+	-	-	-	-	-	-	+	+	-	-	+	+
	eo	+	+	-	-	-	-	+	+	-	-	+	-	+	+	+	-
	oe	+	-	+	-	-	+	-	+	-	+	+	+	-	+	-	-
	oo	+	-	-	+	-	+	+	-	-	+	+	-	+	-	-	+
SS	ee	+	+	+	+	+	+	+	+	-	-	-	-	-	-	-	-
	eo	+	+	-	-	+	+	-	-	-	-	-	+	+	+	-	+
	oe	+	-	+	-	+	-	+	-	-	+	-	-	-	+	+	+
	oo	+	-	-	+	+	-	-	+	-	+	-	+	+	-	+	-

If the group $p6mm$ is referred to the orthohexagonal axes $A=a_1+a_2$, $B=a_1-a_2$, the applicable plane group will be $c2mm$, for which the elimination table reads

	$g'm'$ 2 2'	$g m$ 2 2'	$g m$ $m'g'$
$c g'$ $g 2'$	$c m'$ 2 g	$c m$ 2 g'	$c m$ $m'2'$
$c g'$ $g 2'$	$c m'$ 2 g	$c m$ 2 g'	$c m$ $m'2'$
	$g'm'$ 2 2'	$g m$ 2 2'	$g m$ $m'g'$

There will be two terms to sum, and if the series is summed for one-eighth of the cell, as is usual for $c2mm$, three asymmetric units of the $p6mm$ will be obtained. However, in this case the lattices for the three sub-units will not necessarily coincide with respect to the orthohexagonal cell. However, if data are combined from the three representations of the

hexagonal asymmetric unit, values can be obtained on some points of a mesh finer than that originally computed.

M. J. Buerger (*Am. Min.*, 34, 771-88, 1949) has suggested a different approach to the computation of plane groups having 3, 4 and 6 axes. He suggests making an asymmetric or centrosymmetric computation for the whole or half-cell, using only the "asymmetric unit" of the data in reciprocal space. He then develops the full symmetry by appropriate recombination procedures. Further details must be obtained from the original paper.

2.5.4.9. FOURIER SERIES IN THREE DIMENSIONS

The most general Fourier series in three dimensions is of the form

$$f(x, y, z) = \sum_{h,k,l} F(hkl) e^{-2\pi i(hx+ky+lz)} \quad \dots (34a)$$

in which

$$F(h, k, l) = \int_0^1 \int_0^1 \int_0^1 f(x, y, z) e^{2\pi i(hx+ky+lz)} dx dy dz \quad \dots (34b)$$

The Fourier coefficients are in general complex and may be written

$$F(hkl) = A(hkl) + iB(hkl) \quad \dots (35)$$

If $f(x, y, z)$ is real, we have

$$F(hkl) = \tilde{F}(\bar{h}\bar{k}\bar{l}) \quad \dots (36)$$

$$\text{i.e. } A(h, k, l) = A(\bar{h}, \bar{k}, \bar{l}) \text{ and } B(hkl) = -B(\bar{h}, \bar{k}, \bar{l}) \quad \dots (37)$$

The series (34a) can be written in the form

$$f(x, y, z) = \sum_{h,k,l=-\infty}^{\infty} \{A(h, k, l) \cos 2\pi(hx + ky + lz) + B(hkl) \sin 2\pi(hx + ky + lz)\} \quad \dots (38)$$

In general the Fourier coefficients can be evaluated by generalization of one-dimensional methods. For the expansion of a three-dimensional summation in terms of one-dimensional summations see Section 6.5.1. Unfortunately the method of discontinuities has not yet been generalized for the three-dimensional case (see 2.5.4.4(b), page 75). The result of 2.5.4.4(a) can, however, be directly generalized to two or three dimensions as follows:

Consider the triplet $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ and its reciprocal triplet $\mathbf{a}_1^*, \mathbf{a}_2^*, \mathbf{a}_3^*$. Let $\phi_0(\mathbf{x})$ be an arbitrary function of $\mathbf{x} = x_1\mathbf{a}_1 + x_2\mathbf{a}_2 + x_3\mathbf{a}_3$ and $\Phi_0(\mathbf{u})$ be the transform of $\phi_0(\mathbf{x})$, where $\mathbf{u} = u_1\mathbf{a}_1^* + u_2\mathbf{a}_2^* + u_3\mathbf{a}_3^*$ (2.5.3.3 (page 71)). Now define the vector $\mathbf{n} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$, where the n_i are integers, positive, negative or zero. Then consider

$$\begin{aligned} \phi(\mathbf{x}) &= \sum_{n_i=-\infty}^{\infty} \sum_{n_i=-\infty}^{\infty} \sum_{n_i=-\infty}^{\infty} \phi_0(\mathbf{x} - \mathbf{n}) \\ &= \frac{1}{V} \sum_{h_i=-\infty}^{\infty} \sum_{h_i=-\infty}^{\infty} \sum_{h_i=-\infty}^{\infty} \Phi(h_1h_2h_3) e^{-2\pi i(h_1x_1 + h_2x_2 + h_3x_3)} \quad \dots (39) \end{aligned}$$

It then follows that†

$$\begin{aligned} \Phi(h_1h_2h_3) &= \frac{1}{V} \int_0^1 \int_0^1 \int_0^1 \phi(\mathbf{x}) e^{2\pi i\mathbf{h}\cdot\mathbf{x}} dx_1 dx_2 dx_3 \\ &= \frac{1}{V} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \phi_0(\mathbf{x}) e^{2\pi i\mathbf{h}\cdot\mathbf{x}} dx_1 dx_2 dx_3 = \frac{1}{V} \Phi_0(\mathbf{h}) \quad \dots (40) \end{aligned}$$

in which $\mathbf{h} = h_1\mathbf{a}_1^* + h_2\mathbf{a}_2^* + h_3\mathbf{a}_3^*$. The Fourier coefficients are thus given directly by sampling the transform $\Phi_0(\mathbf{u})$ of $\phi_0(\mathbf{x})$ at the whole-numbered points $\mathbf{u}_i = \mathbf{h}_i$.

A particularly important case arises in which ϕ_0 is a function only of the radius $r = |\mathbf{x}|$ given by $|\mathbf{x}|^2 = \sum \sum (\mathbf{a}_i \mathbf{a}_j) x_i x_j$. In this case $\Phi(h_1h_2h_3) = \Phi(\mathbf{h}) = \Phi(|\mathbf{h}|)$ and $|\mathbf{h}|^2 = \sum \sum h_i h_j (\mathbf{a}_i^* \mathbf{a}_j^*)$. We then have by 2.5.3.3 (19b):

$$\Phi(|\mathbf{h}|) = \frac{4\pi}{V} \int_0^{\infty} \phi_0(r) \frac{\sin 2\pi r |\mathbf{h}|}{2\pi r |\mathbf{h}|} r^2 dr \quad \dots (41)$$

in which V is the unit cell volume of the triplet \mathbf{a}_i .

2.5.4.10. PROPERTIES OF CONVOLUTIONS

The eight formulae represented by entries 8.1, 8.2, 9.1, 9.2 of Table 2.5.3A are referred to as convolutions of the functions $f(x)$ and $g(x)$ with one another or of $F(u)$ and $G(u)$ with one another. The German word *Faltung* and its English equivalents “fold” or “folding” have also been used as synonyms for “convolution.”

If it is assumed that $f(x)$ and $g(x)$ are complex functions of the real variable x , which may be assumed to be a real variable vector in one or more dimensions, there are sixty-four convolution formulae which may be derived from formulae 8.1 and 9.1 of Table 2.5.3A by successive application of formulae 4 and 7 of that table. Table 2.5.4D lists the sixteen essentially different transforms which can be obtained from such formulae together with two possible forms for the integrand of the convolution. Two additional forms can be obtained by changing the sign of the running variable η in the integrands tabulated. The column headed “Reduced Form” will be referred to below. The corresponding convolutions in transform space are identical in form with those in the base space and are readily obtained from the table as indicated in the notes to the table. Any entry in the table can be readily verified as follows. One of the integrands of the first entry of the second block of the table gives rise to

$$\begin{aligned} \int f(x + \eta) \tilde{g}(\eta) d\eta &= \int \int F(u) e^{-2\pi i u(x + \eta)} \tilde{g}(\eta) du d\eta \\ &= \int F(u) e^{-2\pi i u x} \int \tilde{g}(\eta) e^{-2\pi i u \eta} d\eta du = \int F(u) \tilde{G}(u) e^{-2\pi i u x} du \end{aligned}$$

which verifies the entry in the table.

In dealing with real functions f and g it should be remembered that $F(\bar{u}) = \tilde{F}(u)$. There are then only sixteen forms for the convolution instead of sixty-four.

In many of the applications in X-ray crystallography the two functions f and g are equal. In such *auto-convolutions* there are clearly ten different transforms, which are listed in Table 2.5.4E. This table is also grouped to indicate the three different forms which are assumed by the auto-convolutions of real functions.

The column of Table 2.5.4D headed “Reduced Form” indicates that all sixteen types of convolution can be interpreted in the same way as a correlation between the weights of the two functions at points separated by a distance x . In Figure 2.5.4 two identical infinitesimals $d\eta$ (length, area or volume) are located at $(\eta + \frac{1}{2}x)$ and $(\eta - \frac{1}{2}x)$. The convolution then measures the product of the weights of two functions at the two infinitesimals multiplied by the common infinitesimal and summed over all values of η . Both functions are referred to the same origin, but for a given convolution the function referred to that origin and a particular infinitesimal may be the function itself or its inverse

† Note that we have varied the technique from that of 2.5.4.4(a) (page 75) by defining $\phi_0(\mathbf{x})$ and $\Phi_0(\mathbf{u})$ in terms of the system \mathbf{a}_i and \mathbf{a}_i^* instead of in terms of a unit system as before. Both procedures are equally valid.

TABLE 2.5.4D
Forms for the Convolution Formulae

NOTE 1. The first entry corresponds to

$$\int F(u)G(u)e^{-2\pi iux} du = \int f(\eta)g(x-\eta)d\eta = \int f(x-\eta)g(\eta)d\eta \\ = \int f(-\eta)g(x+\eta)d\eta = \int f(x+\eta)g(-\eta)d\eta$$

The third and fourth convolutions are obtained from those given in the table by changing the sign of η .

NOTE 2. An overrule indicates a negative quantity.

NOTE 3. Convolutions in transform space are obtained by interchanging the variables x and u and interchanging capital and small letters.

Transforms	Convolution Integrands		Reduced Form
$F(u)G(u)$	$f(\eta)g(x-\eta)$	$f(x-\eta)g(\eta)$	$f(\eta+\frac{1}{2}x)g(\eta-\frac{1}{2}x)$
$F(u)G(\bar{u})$	$f(\eta)g(\overline{x-\eta})$	$f(x-\eta)g(\bar{\eta})$	$f(\eta+\frac{1}{2}x)g(\eta-\frac{1}{2}x)$
$F(\bar{u})G(u)$	$f(\bar{\eta})g(x-\eta)$	$f(\overline{x-\eta})g(\eta)$	$f(\eta-\frac{1}{2}x)g(\eta+\frac{1}{2}x)$
$F(\bar{u})G(\bar{u})$	$f(\bar{\eta})g(\overline{x-\eta})$	$f(\overline{x-\eta})g(\bar{\eta})$	$f(\eta+\frac{1}{2}x)g(\eta-\frac{1}{2}x)$
$F(u)\tilde{G}(u)$	$f(\eta)\tilde{g}(\overline{x-\eta})$	$f(x-\eta)\tilde{g}(\bar{\eta})$	$f(\eta+\frac{1}{2}x)\tilde{g}(\eta-\frac{1}{2}x)$
$F(u)\tilde{G}(\bar{u})$	$f(\eta)\tilde{g}(x-\eta)$	$f(x-\eta)\tilde{g}(\eta)$	$f(\eta+\frac{1}{2}x)\tilde{g}(\eta-\frac{1}{2}x)$
$F(\bar{u})\tilde{G}(u)$	$f(\bar{\eta})\tilde{g}(\overline{x-\eta})$	$f(\overline{x-\eta})\tilde{g}(\bar{\eta})$	$f(\eta+\frac{1}{2}x)\tilde{g}(\eta-\frac{1}{2}x)$
$F(\bar{u})\tilde{G}(\bar{u})$	$f(\bar{\eta})\tilde{g}(x-\eta)$	$f(\overline{x-\eta})\tilde{g}(\eta)$	$f(\eta-\frac{1}{2}x)\tilde{g}(\eta+\frac{1}{2}x)$
$\tilde{F}(u)G(u)$, etc.	Interchange f and g in preceding block		
$\tilde{F}(u)\tilde{G}(u)$	$\tilde{f}(\bar{\eta})\tilde{g}(\overline{x-\eta})$	$\tilde{f}(\overline{x-\eta})\tilde{g}(\bar{\eta})$	$\tilde{f}(\eta+\frac{1}{2}x)\tilde{g}(\eta-\frac{1}{2}x)$
$\tilde{F}(u)\tilde{G}(\bar{u})$	$\tilde{f}(\bar{\eta})\tilde{g}(x-\eta)$	$\tilde{f}(\overline{x-\eta})\tilde{g}(\eta)$	$\tilde{f}(\eta-\frac{1}{2}x)\tilde{g}(\eta+\frac{1}{2}x)$
$\tilde{F}(\bar{u})\tilde{G}(u)$	$\tilde{f}(\eta)\tilde{g}(\overline{x-\eta})$	$\tilde{f}(x-\eta)\tilde{g}(\bar{\eta})$	$\tilde{f}(\eta+\frac{1}{2}x)\tilde{g}(\eta-\frac{1}{2}x)$
$\tilde{F}(\bar{u})\tilde{G}(\bar{u})$	$\tilde{f}(\eta)\tilde{g}(x-\eta)$	$\tilde{f}(x-\eta)\tilde{g}(\eta)$	$\tilde{f}(\eta+\frac{1}{2}x)\tilde{g}(\eta-\frac{1}{2}x)$

TABLE 2.5.4E
Forms for Auto-convolutions

NOTE. The entries in each block reduce to the same form for real functions, in which case the first two blocks are inverses of one another.

Transform	Convolution Integrands			
$F^2(u)$	$f(\eta)f(x-\eta)$	$f(\bar{\eta})f(x+\eta)$		
$F(u)\tilde{F}(\bar{u})$	$f(\eta)\tilde{f}(x-\eta)$	$f(\bar{\eta})\tilde{f}(x+\eta)$	$f(x-\eta)\tilde{f}(\eta)$	$f(x+\eta)\tilde{f}(\bar{\eta})$
$\tilde{F}^2(\bar{u})$	$\tilde{f}(\eta)\tilde{f}(x-\eta)$	$\tilde{f}(\bar{\eta})\tilde{f}(x+\eta)$		
$F^2(\bar{u})$	$f(\bar{\eta})f(\overline{x-\eta})$	$f(\eta)f(\overline{x+\eta})$		
$F(\bar{u})\tilde{F}(u)$	$f(\bar{\eta})\tilde{f}(\overline{x-\eta})$	$f(\eta)\tilde{f}(\overline{x+\eta})$	$f(\overline{x-\eta})\tilde{f}(\bar{\eta})$	$f(\overline{x+\eta})\tilde{f}(\eta)$
$\tilde{F}^2(u)$	$\tilde{f}(\bar{\eta})\tilde{f}(\overline{x-\eta})$	$\tilde{f}(\eta)\tilde{f}(\overline{x+\eta})$		
$ F(u) ^2$	$f(\eta)\tilde{f}(\overline{x-\eta})$	$f(\bar{\eta})\tilde{f}(\overline{x+\eta})$	$f(x-\eta)\tilde{f}(\bar{\eta})$	$f(x+\eta)\tilde{f}(\eta)$
$F(u)F(\bar{u})$	$f(\eta)f(\overline{x-\eta})$	$f(\bar{\eta})f(\overline{x+\eta})$	$f(x-\eta)f(\bar{\eta})$	$f(x+\eta)f(\eta)$
$\tilde{F}(u)\tilde{F}(\bar{u})$	$\tilde{f}(\bar{\eta})\tilde{f}(x-\eta)$	$\tilde{f}(\eta)\tilde{f}(x+\eta)$	$\tilde{f}(\overline{x-\eta})\tilde{f}(\eta)$	$\tilde{f}(\overline{x+\eta})\tilde{f}(\bar{\eta})$
$ F(\bar{u}) ^2$	$f(\bar{\eta})\tilde{f}(x-\eta)$	$f(\eta)\tilde{f}(x+\eta)$	$f(\overline{x+\eta})\tilde{f}(\eta)$	$f(x-\eta)\tilde{f}(\bar{\eta})$

in the origin or its conjugate complex. It must be emphasized that this geometrical interpretation is only one of many possible. Still more generalized types of convolution may be set up (Patterson [58]) in which the correlation expressed by Fig. 2.5.4 is carried out between a function and those related to it by any of the crystallographic symmetry operations.

In discussion of Fourier transforms all convolution integrals are doubly infinite, while for periodic functions the integrals are usually taken over a single cell.

The most important applications of the convolution formulae to crystallography depend on the properties of "atomic functions" (2.5.3.2 (a), page 70).

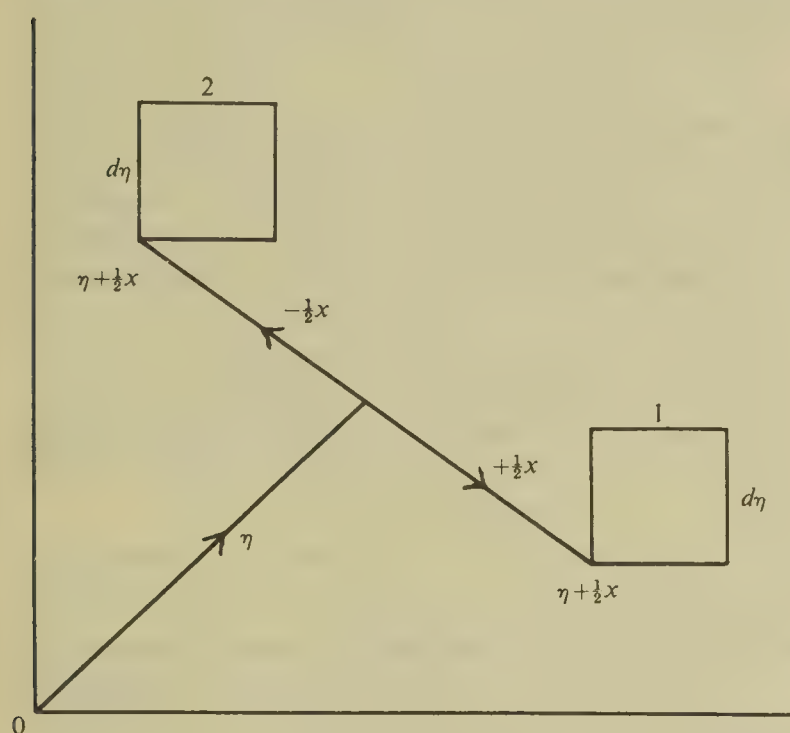


Fig. 2.5.4

Assume that $f(x)$, $g(x)$ are of the form

$$f(x) = \sum_1^M f_i(x - a_i) \quad \text{and} \quad g(x) = \sum_1^N g_i(x - b_i) \quad \dots (42)$$

Then, by 2.5.3.2 (13) (p. 70), the transforms $F(u)$ and $G(u)$ are given by

$$F(u) = \sum_1^M F_i(u) e^{2\pi i u a_i} \quad \text{and} \quad G(u) = \sum_1^N G_i(u) e^{2\pi i u b_i} \quad \dots (43)$$

in which the functions $F_i(u)$ are the transforms of the individual functions $f_i(x)$, etc. For such functions the convolutions can be written as the various possible products of the two functions (43) and their conjugates and inverses. Table 2.5.4F lists the expressions corresponding to the first four entries of Table 2.5.4D. The products corresponding to the remaining twelve entries of Table 2.5.4D can be written down by inspection. From Table 2.5.4F we can make the following statement. The convolution of two functions f and g which are the sum of M and N atomic functions respectively will consist of MN atomic functions located at origins whose co-ordinates will be sums or differences of the co-ordinates of the origins in the original functions. The convolution atomic functions will be convolutions pairwise of the original atomic functions.

In addition to the application of the convolution in the calculation of vector maps (Section 6.1, page 318) it has also proved of importance in the calculation of molecular transforms and in the calculation of diffraction from small crystal particles (Section 6.3, page 322).

TABLE 2.5.4F

Convolutions of "Atomic Functions"

$$\text{Typical Case: } F(u)G(u) = \sum_{i=1}^M \sum_{j=1}^N F_i(u)G_j(u) e^{2\pi i u(a_i + b_j)}$$

The table lists transforms of convolution atomic functions (e.g. $F_i(u)G_j(u)$) and locations of the corresponding convolution atomic functions (e.g. $a_i + b_j$).

Transforms	Transforms of Convolution Atomic Functions	Location of Convolution Atomic Functions
$F(u)G(u)$	$F_i(u)G_j(u)$	$a_i + b_j$
$F(u)G(\bar{u})$	$F_i(u)G_j(\bar{u})$	$a_i - b_j$
$F(\bar{u})G(u)$	$F_i(\bar{u})G_j(u)$	$-a_i + b_j$
$F(\bar{u})G(\bar{u})$	$F_i(\bar{u})G_j(\bar{u})$	$-a_i - b_j$

2.6. Statistics

By D. W. J. CRUICKSHANK

2.6.1. Introduction

2.6.1.1. GENERAL INTRODUCTION

The assessment of the accuracy of a measurement or of quantities derived from measurements is a cardinal problem in every experimental science. No measurement is of any value unless one has at least some idea of its accuracy.

A single measurement of the magnitude of a quantity differs by errors from its unknown true value λ . The fundamental supposition usually made about the errors is that, for a given experimental procedure, the possible results of an experiment define the probability distribution of a random variable ξ . If, for instance, the random variable has a continuous range of values x , it is supposed that there is a probability density function $f(x)$ such that $f(x)dx$ is the probability of a single measurement lying in the range $(x, x+dx)$. Both the true value λ and the probability density $f(x)$ are unknown. The problem of assessing the accuracy of a measurement is thus the double problem of estimating $f(x)$ and of assuming a relation between $f(x)$ and λ .

For many purposes the crudest of estimates of $f(x)$ may suffice—a mere glance at a measuring scale may be adequate to determine limits of error—but for work of precision more formal methods are needed. Fortunately the theory of probability shows that it is often unnecessary to estimate the complete form of $f(x)$. It is commonly sufficient to estimate only the mean and the variance of the distribution. These estimates can be made in a straightforward manner from the results of a series of experiments.

The problem of what relation to assume between $f(x)$ and the true value λ is a more subtle one, involving particularly the question of systematic errors. The usual procedure, after correction for known systematic errors, is to suppose that some typical value of $f(x)$, ordinarily the mean, is the value of λ . No repetition of an experiment will ever reveal the systematic errors, so that statistical estimates of accuracy take into account only the random errors. Empirically, systematic errors can be detected only by remeasuring the quantity with a different technique.

In the preceding remarks the concepts of probability have been applied to the errors of measurements. This kind of application is frequently needed in the physical sciences. The situation in the biological sciences is rather different: here the errors in the measurements themselves are often negligible and the concepts of probability are applied to samples from populations of plants and animals, each individual in the population being regarded as giving a measure of the property of interest. In these applications the concept of a unique true value of a quantity has no place; the usual

conception is that of an ideal infinite population such that $f(x)dx$ is the probability of a member of the population having the property with a value in the range $(x, x+dx)$. Similar conceptions occur in the basic applications of probability in quantum mechanics.

For definiteness the applications of the theory of probability in the following sections are described in terms of the assessment of the accuracy of measurements, but the methods are often applicable in population problems.

In the hope that it will ease the task of any reader who wishes to study a point in more detail, an attempt has been made to follow, in a general way, the style of one of the standard texts. Accordingly the definitions, notation and sequence of the mathematical matter in these sections are rather similar to those used by Cramér in *The Elements of Probability Theory* [67] and *Mathematical Methods of Statistics* [68]. No blame is, of course, to be attached to Cramér for any mistakes made here; in any case the present treatment differs from his in a number of important respects.

2.6.1.2. FUNDAMENTAL RULES FOR COMBINING PROBABILITIES

- (a) The probability that one of several mutually exclusive events will happen is the sum of the separate probabilities.
- (b) The probability of the combined occurrence of two events, S and T , is the product of the probability of S and of the (conditional) probability of T on the assumption that S has happened; or alternatively it is the product of the probability of T and of the (conditional) probability of S on the assumption that T has happened.

Hence, if the events are independent, the probability of the combined occurrence is the product of the probabilities of the separate events.

2.6.2. One-dimensional Probability Distributions

2.6.2.1. DISCRETE AND CONTINUOUS DISTRIBUTIONS

The two simple types of one-dimensional probability distribution are the *discrete*, in which the random variable ξ takes only certain discrete values, and the *continuous*, in which both the range and the probability distribution of the random variable are continuous (though the range may be bounded).

For a discrete probability distribution let p_i be the probability that ξ will take the value x_i . The normalization condition is

$$\sum_i p_i = 1 \quad \dots (1)$$

where the summation is over all possible values of i .

For a continuous probability distribution let $f(x)dx$ be the probability that ξ will take a value between x and $x+dx$. The normalization condition is

$$\int_a^b f(x)dx = 1 \quad \dots (2a)$$

where a and b are the limiting values of ξ . By defining $f(x)=0$ outside the range $a \leq x \leq b$, this may alternatively be written

$$\int_{-\infty}^{\infty} f(x)dx = 1 \quad \dots (2b)$$

The *mean value*, or the *expected value*, of a function $g(\xi)$ of the random variable ξ is defined as

$$E\{g(\xi)\} = \sum_i g(x_i)p_i \quad \text{or} \quad \int_{-\infty}^{\infty} g(x)f(x)dx \quad \dots (3)$$

for discrete and continuous distributions respectively.

In particular, the *mean* m of a distribution is

$$m \equiv E(\xi) = \sum_i x_i p_i \quad \text{or} \quad \int_{-\infty}^{\infty} x f(x)dx \quad \dots (4)$$

Also, if a and b are constant:

$$E(a\xi + b) = aE(\xi) + b \quad \dots (5a)$$

further, since $E(\xi) = m$:

$$E(\xi - m) = 0 \quad \dots (5b)$$

Theorem. If ξ and η are random variables, whether independent or not:

$$E(\xi + \eta) = E(\xi) + E(\eta) \quad \dots (6)$$

Theorem. If ξ and η are independent random variables:

$$E(\xi\eta) = E(\xi)E(\eta) \quad \dots (7)$$

2.6.2.2. MOMENTS

If r is a non-negative integer, the *moment of order r* of the random variable ξ is

$$\alpha_r \equiv E(\xi^r) = \sum_i x_i^r p_i \quad \text{or} \quad \int_{-\infty}^{\infty} x^r f(x)dx \quad \dots (8)$$

$\alpha_0 = 1$ is a consequence of the normalization condition, while $\alpha_1 = m$, the mean.

The *central moments* are the moments about the mean m and are

$$\mu_r \equiv E\{(\xi - m)^r\} = \sum_i (x_i - m)^r p_i \quad \text{or} \quad \int_{-\infty}^{\infty} (x - m)^r f(x)dx \quad \dots (9)$$

The relations between the moments about the origin and the central moments are

$$\mu_0 = \alpha_0 = 1; \mu_1 = 0; \mu_2 = \alpha_2 - m^2 \quad \dots (10a)$$

and generally

$$\mu_r = \alpha_r - \binom{r}{1} m \alpha_{r-1} + \binom{r}{2} m^2 \alpha_{r-2} - \dots \quad \dots (10b)$$

2.6.2.3. MEASURES OF LOCATION

The three most important measures of a typical property of a distribution are the *mean*, the *median* and the *mode*, of which the mean has already been defined.

The *median* of a continuous distribution is the value x_0 such that

$$\int_{-\infty}^{x_0} f(x)dx = \frac{1}{2} = \int_{x_0}^{\infty} f(x)dx \quad \dots (11a)$$

For a discrete distribution let the possible values x_i of ξ be arranged in ascending order. Then, if x_j is a value such that

$$\sum_{i=1}^{j-1} p_i < \frac{1}{2} \quad \text{and} \quad \sum_{i=1}^j p_i > \frac{1}{2} \quad \dots (11b)$$

x_j is the *median* of the discrete distribution. If, however,

$$\sum_{i=1}^j p_i = \frac{1}{2} \quad \dots (11c)$$

the median is any value between x_j and x_{j+1} .

The *modes* of a distribution are those values of x at which $f(x)$ or p_i have maxima. If there is only one mode, the distribution is *unimodal*.

2.6.2.4. MEASURES OF DISPERSION

The second moment about the origin α_2 is sometimes called the *mean square deviation*, and its square root the *root mean square deviation*.

The second order central moment μ_2 is the *variance*, and its positive square root is the *standard deviation* (s.d.) σ .

The *lower quartile* of a continuous distribution is that value x_l for which

$$\int_{-\infty}^{x_l} f(x)dx = \frac{1}{4} \quad \dots (12a)$$

while the *upper quartile* is that value x_u for which

$$\int_{x_u}^{\infty} f(x)dx = \frac{1}{4} \quad \dots (12b)$$

The *semi-interquartile range* is $\frac{1}{2}(x_u - x_l)$; in a symmetrical distribution this is sometimes (and somewhat misleadingly) called the *probable error*.

2.6.2.5. MEASURES OF SKEWNESS

A distribution is *symmetric* if it is symmetric about the mean. In a symmetric distribution all the central moments of odd order, μ_{2n+1} , vanish.

The third order central moment μ_3 is one of the simplest measures of skewness. The dimensionless quantity μ_3/σ^3 is sometimes called the *coefficient of skewness*.

For unimodal continuous distributions of small skewness the relation

$$\text{Mean} - \text{mode} = 3(\text{mean} - \text{median}) \quad \dots (13)$$

holds approximately.

Karl Pearson's definition of skewness is

$$\text{Skewness} = \frac{\text{mean} - \text{mode}}{\sigma}$$

The continuous distribution shown in Fig. 2.6.2.5 exhibits positive skewness.

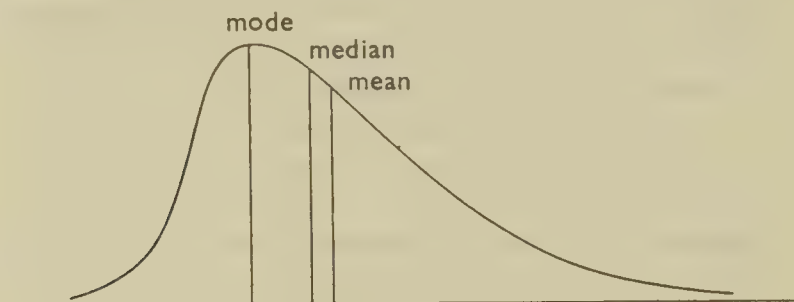


Fig. 2.6.2.5

2.6.2.6. CHARACTERISTIC FUNCTIONS

The mean value of the random variable $e^{it\xi}$ may be written

$$\phi(t) = E(e^{it\xi}) = \sum_i e^{itx_i} p_i \quad \text{or} \quad \int_{-\infty}^{\infty} e^{itx} f(x) dx \quad \dots (14)$$

This function of the real variable t is called the *characteristic function* of the distribution $f(x)$. Apart from a factor 2π it is the Fourier transform of the distribution.

The theoretical importance of characteristic functions arises as follows. The probability distribution $f(x)$ of the sum of two independent random variables ξ and η is the convolution of their respective distributions $f_1(x)$ and $f_2(x)$, thus

$$f(x) = \int_{-\infty}^{\infty} f_1(x-z) f_2(z) dz = \int_{-\infty}^{\infty} f_2(x-z) f_1(z) dz \quad \dots (15)$$

Hence by the convolution theorem, Section 2.5.3.1, the characteristic function $\phi(t)$ of $(\xi + \eta)$ is the product of the characteristic functions $\phi_1(t)$ of ξ and $\phi_2(t)$ of η . More generally, the characteristic function of a sum of independent variables is equal to the product of the characteristic functions of the variables.

The probability distribution of a sum of independent variables may thus be found by taking the Fourier transforms of the individual distributions, multiplying these transforms together and then taking the inverse Fourier transform to obtain the probability distribution of the sum.

Assuming the moments exist, the sum or integral defining the characteristic function may be expanded for small values of t to give

$$\phi(t) = 1 + \sum_{r=1}^{\infty} \frac{\alpha_r}{r!} (it)^r \quad \dots (16)$$

where the α_r are the moments.

The corresponding expansion of $\log \phi(t)$ defines the *semi-invariants* or *cumulants* κ_r

$$\log \phi(t) = \sum_{r=1}^{\infty} \frac{\kappa_r}{r!} (it)^r \quad \dots (17)$$

If $\phi(t)$ is the characteristic function of a sum of independent random variables with characteristic functions $\phi_1(t)$, $\phi_2(t)$, \dots , $\phi_n(t)$ the convolution theorem gives

$$\log \phi(t) = \log \phi_1(t) + \log \phi_2(t) + \dots + \log \phi_n(t) \quad \dots (18)$$

and hence the r th semi-invariant of the sum is the sum of the r th semi-invariants of the individual distributions

$$\kappa_r = \kappa_r^{(1)} + \kappa_r^{(2)} + \dots + \kappa_r^{(n)} \quad \dots (19)$$

This relation is the chief reason for the introduction of semi-invariants; no corresponding relation holds in general for the central moments except for the first three:

$$\left. \begin{aligned} m &= m_1 + m_2 + \dots + m_n \\ \sigma^2 &= \sigma_1^2 + \sigma_2^2 + \dots + \sigma_n^2 \\ \mu_3 &= \mu_3^{(1)} + \mu_3^{(2)} + \dots + \mu_3^{(n)} \end{aligned} \right\} \quad \dots (20)$$

The first few relations between the semi-invariants and the moments are

$$\left. \begin{aligned} \kappa_1 &= \alpha_1 = m \\ \kappa_2 &= \alpha_2 - \alpha_1^2 = \sigma^2 \\ \kappa_3 &= \alpha_3 - 3\alpha_1\alpha_2 + 2\alpha_1^3 \end{aligned} \right\} \quad \dots (21)$$

The first few relations between the semi-invariants and the central moments are

$$\left. \begin{aligned} \kappa_1 &= m \\ \kappa_2 &= \mu_2 = \sigma^2 \\ \kappa_3 &= \mu_3 \\ \kappa_4 &= \mu_4 - 3\mu_2^2 \end{aligned} \right\} \quad \dots (22)$$

2.6.3. Particular One-dimensional Distributions

2.6.3.1. THE BINOMIAL DISTRIBUTION

Let p be the constant chance of an event in a random experiment, and let $q = 1 - p$. The probability of the event occurring r times in n repetitions of the experiment is

$$\binom{n}{r} p^r q^{n-r} \quad \dots (1)$$

The corresponding probability distribution in which the variate takes the values $0, 1, 2, \dots, r, \dots, n$ with probabilities

$$q^n, nq^{n-1}p, \dots, \binom{n}{r} p^r q^{n-r}, \dots, p^n$$

is the *binomial distribution*; it is so called because these probabilities are the successive terms in the binomial expansion of $(p+q)^n$.

The mean of the distribution is $m = np$; the variance $\sigma^2 = \mu_2 = npq$, and $\mu_3 = npq(q-p)$.

2.6.3.2. POISSON'S DISTRIBUTION

In *Poisson's distribution* with parameter λ the random variable takes the values $0, 1, 2, 3, \dots, r, \dots (\infty)$ with probabilities

$$e^{-\lambda}, \lambda e^{-\lambda}, \frac{\lambda^2}{2!} e^{-\lambda}, \frac{\lambda^3}{3!} e^{-\lambda}, \dots, \frac{\lambda^r}{r!} e^{-\lambda}, \dots$$

The distribution may be regarded as a limiting form of the binomial distribution in which $n \rightarrow \infty$ and $p = \lambda/n$. It is thus applicable to problems involving a large number of experiments, in each of which there is a constant small chance of an event occurring, or to problems including a large number of individuals, to each of whom there is a constant small chance of some happening.

All the semi-invariants of the distribution are equal to λ , so that $m = \lambda$, $\sigma^2 = \lambda$ and $\mu_3 = \lambda$.

The sum of any finite number of independent Poissonian variables is itself a Poissonian variable, with parameter λ equal to the sum of the parameters $\lambda_1, \lambda_2, \dots$ of the separate variables.

2.6.3.3(a). THE NORMAL DISTRIBUTION

A random variable ξ is *normally distributed* if it has a probability distribution

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-m)^2}{2\sigma^2}\right) \quad \dots (2)$$

This distribution is symmetrical about its mean m and it has variance σ^2 . The mean, median and mode of the distribution are coincident.

The *mean deviation*, $E(|\xi - m|)$, from the mean of a normal variate is

$$\sqrt{\frac{2}{\pi}} \sigma = 0.7979\sigma$$

The *semi-interquartile range* or *probable error* (Section 2.6.2.4) of a normal variate is 0.6745σ .

Theorem. If the set of random variables ξ_i ($i=1, 2, \dots, n$) are independent and normally distributed with means m_i and variances σ_i^2 , the variable

$$\xi = a_1\xi_1 + a_2\xi_2 + \dots + a_n\xi_n \quad \dots (3)$$

is normally distributed with mean

$$m = a_1m_1 + a_2m_2 + \dots + a_nm_n \quad \dots (4)$$

and with variance

$$\sigma^2 = a_1^2\sigma_1^2 + a_2^2\sigma_2^2 + \dots + a_n^2\sigma_n^2 \quad \dots (5)$$

Theorem. In particular, if the independent variables are normally distributed with a common mean m and a common variance σ^2 , their arithmetic mean is also normally distributed about m with variance σ^2/n .

2.6.3.3(b). THE CENTRAL LIMIT THEOREM

The great theoretical importance of the normal distribution arises from the *Central Limit Theorem*, which may be stated as:

Whatever the distribution of the independent

variables ξ_i —subject to certain very general conditions—the distribution of the sum

$$\xi = \xi_1 + \xi_2 + \dots + \xi_n \quad \dots (6)$$

tends to the normal distribution, as $n \rightarrow \infty$, with mean

$$m = m_1 + m_2 + \dots + m_n \quad \dots (7)$$

and variance

$$\sigma^2 = \sigma_1^2 + \sigma_2^2 + \dots + \sigma_n^2 \quad \dots (8)$$

Discussion of these very general conditions will be found in Cramér, *Mathematical Methods of Statistics*; Kendall, *Advanced Theory of Statistics*, etc., but, roughly speaking, the only requirements are that each ξ_i must have a finite variance, and the probability of any ξ_i making a relatively large contribution to the total value of ξ must be small.

The Central Limit Theorem makes it plausible to suppose that if the experimental determination of the value of a quantity is subject to a large number of independent sources of small errors, the probability distribution of the quantity will be normal. This may be considered the explanation of the fact that observed distributions are often approximately normal.

2.6.3.4. THE χ^2 DISTRIBUTION

Let $\xi_1, \xi_2, \dots, \xi_n$ be n independent random variables, each normally distributed with mean 0 and variance 1. The distribution (for $x > 0$) of

$$\chi^2 = \sum_{i=1}^n \xi_i^2$$

is

$$f(x) = \frac{1}{2^{\frac{n}{2}} \Gamma\left(\frac{n}{2}\right)} x^{\frac{n}{2}-1} e^{-\frac{x}{2}} \quad \dots (9)$$

This is known as the χ^2 distribution with n degrees of freedom.

The mean $m = n$ and the variance $\sigma^2 = 2n$.

2.6.3.5. THE t DISTRIBUTION, OR STUDENT'S DISTRIBUTION

If ξ and ξ_1, \dots, ξ_n are $n+1$ independent random variables each normally distributed with mean 0 and variance 1, and if

$$\eta = \left(\sum_{i=1}^n \xi_i^2 / n \right)^{\frac{1}{2}}$$

the variable

$$t = \frac{\xi}{\eta} = \frac{\xi}{\left(\sum_{i=1}^n \xi_i^2 / n \right)^{\frac{1}{2}}} \quad \dots (10)$$

has the distribution

$$s_n(x) = \frac{1}{(n\pi)^{\frac{1}{2}}} \frac{\Gamma\left(\frac{n+1}{2}\right)}{\Gamma\left(\frac{n}{2}\right)} \left(1 + \frac{x^2}{n}\right)^{-\frac{n+1}{2}} \quad \dots (11)$$

This is known as Student's distribution with n degrees of freedom. As $n \rightarrow \infty$ the distribution tends to the normal distribution with mean 0 and variance 1.

2.6. STATISTICS

2.6.3.6. THE F AND z DISTRIBUTIONS

Let ξ_1, \dots, ξ_m and η_1, \dots, η_n be $m+n$ independent random variables, each normally distributed with mean 0 and variance 1, and let

$$\xi = \sum_{i=1}^m \xi_i^2 \quad \text{and} \quad \eta = \sum_{i=1}^n \eta_i^2$$

The variable

$$F = \frac{\xi/m}{\eta/n} = \frac{\sum_{i=1}^m \xi_i^2/m}{\sum_{i=1}^n \eta_i^2/n} \quad \dots (12)$$

has the distribution (for $x > 0$)

$$f(x) = \frac{\Gamma\left(\frac{m+n}{2}\right)}{\Gamma\left(\frac{m}{2}\right)\Gamma\left(\frac{n}{2}\right)} \frac{x^{\frac{m}{2}-1}}{(mx+n)^{\frac{m+n}{2}}} \quad \dots (13)$$

The corresponding distribution of the variable z defined by $\exp(2z) = F$ is known as Fisher's z distribution.

As $n \rightarrow \infty$ the F distribution tends to the distribution of χ^2/m with m degrees of freedom.

2.6.4. Multi-dimensional Distributions

2.6.4.1(a). TWO-DIMENSIONAL PROBABILITY DISTRIBUTIONS

To avoid repetition we shall consider the probability distribution of two one-dimensional random variables ξ and η , the distribution for simplicity being continuous.

Let $f(x, y)dxdy$ be the joint probability that ξ and η will take values in the ranges $(x, x+dx)$ and $(y, y+dy)$ respectively. The normalization condition is

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(x, y)dxdy = 1 \quad \dots (1)$$

The *mean* or *expected value* of a function $g(\xi, \eta)$ is defined as

$$E\{g(\xi, \eta)\} = \int \int g(x, y)f(x, y)dxdy \quad \dots (2)$$

The *moments* of the distribution are

$$\alpha_{rs} = E(\xi^r, \eta^s) = \int \int x^r y^s f(x, y)dxdy \quad \dots (3)$$

The *mean* of the distribution has the co-ordinates (m_1, m_2) where

$$m_1 = \alpha_{10} = E(\xi) \quad \text{and} \quad m_2 = \alpha_{01} = E(\eta) \quad \dots (4)$$

The *central moments* are the moments about the mean and are

$$\mu_{rs} = E\{(\xi - m_1)^r (\eta - m_2)^s\} \quad \dots (5)$$

In particular $\mu_{10} = \mu_{01} = 0$ and $\mu_{20} = \sigma_1^2$, $\mu_{02} = \sigma_2^2$, where σ_1^2 and σ_2^2 are the variances of ξ and η .

μ_{11} is called the *covariance* of ξ and η .

The *correlation coefficient* of the variables ξ and η is

$$\rho = \frac{\mu_{11}}{\sigma_1 \sigma_2} \quad \dots (6)$$

The relations between the second order moments and the second order central moments are

$$\mu_{20} = \alpha_{20} - m_1^2, \quad \mu_{11} = \alpha_{11} - m_1 m_2, \quad \mu_{02} = \alpha_{02} - m_2^2 \quad \dots (7)$$

The bivariate form of the normal distribution has the probability density

$$f(x, y) = \frac{1}{2\pi\sigma_1\sigma_2(1-\rho^2)^{\frac{1}{2}}} \exp \left\{ -\frac{1}{2} \frac{1}{1-\rho^2} \left(\frac{(x-m_1)^2}{\sigma_1^2} - \frac{2\rho(x-m_1)(y-m_2)}{\sigma_1\sigma_2} + \frac{(y-m_2)^2}{\sigma_2^2} \right) \right\} \quad \dots (8)$$

2.6.4.1(b). REGRESSION CURVES

The *regression curve* of the mean of η on ξ is the locus of the point $\{x, m_2(x)\}$, where $m_2(x)$ is the mean value of η when $\xi = x$, i.e.

$$m_2(x) = \frac{\int_{-\infty}^{\infty} y f(x, y) dy}{\int_{-\infty}^{\infty} f(x, y) dy} \quad \dots (9)$$

The regression curves of η on ξ and of ξ on η coincide only when the probability density is concentrated along a single line.

It is sometimes desirable to fit the regression curves by approximate functions. Thus, we may propose to find the best linear estimate of η in terms of ξ , i.e. to find the linear function $g(\xi) = a + b\xi$, such that

$$E\{\eta - g(\xi)\}^2$$

is least.

We obtain

$$E(\eta - a - b\xi)^2 = \mu_{20}b^2 - 2\mu_{11}b + \mu_{02} + (m_2 - a - bm_1)^2 \quad \dots (10)$$

which is a minimum for

$$b = \frac{\mu_{11}}{\mu_{20}} = \frac{\rho\sigma_2}{\sigma_1} \quad \text{and} \quad a = m_2 - bm_1 \quad \dots (11)$$

b is the *regression coefficient* of η on ξ .

Thus the equation of the mean square regression line of η is

$$\frac{y - m_2}{\sigma_2} = \rho \frac{x - m_1}{\sigma_1} \quad \dots (12)$$

which passes through (m_1, m_2) . Conversely, the mean square regression line of ξ is

$$\frac{y - m_2}{\sigma_2} = \frac{1}{\rho} \frac{x - m_1}{\sigma_1} \quad \dots (13)$$

and the regression coefficient of ξ on η is μ_{11}/μ_{02} .

2.6.4.2. MULTI-DIMENSIONAL PROBABILITY DISTRIBUTIONS

Space does not permit a full discussion of multi-variate probability distributions. We shall consider the probability distribution $f(x_1, x_2, \dots, x_n)$ of n one-dimensional random variables $\xi_1, \xi_2, \dots, \xi_n$.

The *moments* of the distribution are

$$\alpha_{r_1 \dots r_n} = E(\xi_1^{r_1} \dots \xi_n^{r_n}) = \int \dots \int x_1^{r_1} \dots x_n^{r_n} f(x_1, \dots, x_n) dx_1 \dots dx_n \quad \dots (14)$$

where $r_1 + r_2 + \dots + r_n$ is the order of the moment.

The *first order moments* are

$$m_i = \int x_i f(x_1, \dots, x_n) dx_1 \dots dx_n \quad \dots (15)$$

The *central moments* are the moments about the mean $m = (m_1, \dots, m_n)$. The following notation will be used for the *second order central moments*:

$$\left. \begin{aligned} \lambda_{ii} &\equiv \sigma_i^2 = E(\xi_i - m_i)^2 \\ \lambda_{ij} &\equiv \rho_{ij} \sigma_i \sigma_j = E\{(\xi_i - m_i)(\xi_j - m_j)\} \end{aligned} \right\} \quad \dots (16)$$

where ρ_{ij} is the correlation coefficient of ξ_i and ξ_j . Accordingly λ_{ii} is the variance of ξ_i and λ_{ij} the covariance of ξ_i and ξ_j .

The matrix whose elements are λ_{ij} is known as the *variance matrix* or *moment matrix*; it is symmetric and positive definite. The matrix with elements ρ_{ij} ($\rho_{ii} = 1$) is the *correlation matrix*. It is also symmetric and positive definite.

If $\eta = a_1 \xi_1 + a_2 \xi_2 + \dots + a_n \xi_n$, the variance of η is

$$\sum_{i=1}^n \sum_{j=1}^n a_i a_j \lambda_{ij} \quad \dots (17)$$

The multivariate form of the normal distribution has the probability density

$$f(x_1, \dots, x_n) = (2\pi)^{-\frac{1}{2}n} (\det A)^{-\frac{1}{2}} \exp \left\{ -\frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \lambda^{ij} (x_i - m_i)(x_j - m_j) \right\} \quad \dots (18)$$

where $\det A$ is the determinant of the moment matrix of the distribution and λ^{ij} are the elements of the inverse matrix.

2.6.5. Sampling Distributions

2.6.5.1. LARGE SAMPLES

Thus far probability distributions have been considered only in the abstract. We must now return to the problem of the assessment of the accuracy of measurements introduced in Section 2.6.1.1 and to the problem of estimating the probability density appropriate to a particular experiment. A single measurement tells us almost nothing: it is only by repeating the measurement a number of times that we can make some estimate of the distribution $f(x)$.

It is usual, of course, to attempt to neutralize the effects of unknown systematic errors in any apparatus by making further measurements after altering details of the apparatus or, better still, by making additional measurements with other techniques. We shall postpone consideration of such methods until Section 2.6.6.3, as it is more convenient to discuss first the accuracy of results obtained from repeated measurements with the same apparatus. This first discussion necessarily excludes any allowance for systematic errors.

Suppose that the values of a one-dimensional random variable obtained in a sequence of measurements are

$$x_1, x_2, \dots, x_n$$

We shall regard these as a sample of n values from the distribution $f(x)$ appropriate to the experiment. Even if n is rather large this sample will not be sufficient to obtain a reliable estimate of the whole form of $f(x)$. Nevertheless, for large n some very remarkable and important results can be obtained by applying the Central Limit Theorem. In particular, although we know nothing of $f(x)$ in advance, provided only that we can assume that it is a distribution satisfying the very general requirements of the Central Limit Theorem, we can say the distribution of the mean \bar{x} of the sample is normal, with the same mean m as the parent random variable ξ and with variance σ^2/n . To determine the accuracy of the value \bar{x} , which we obtain from the sequence of measurements, we require therefore only to estimate σ^2 .

The variance s^2 of the n values in the sample is

$$s^2 = \frac{1}{n} \sum_i (x_i - \bar{x})^2 \quad \dots (1)$$

It may be shown that

$$E(s^2) = \frac{n-1}{n} \sigma^2 \quad \dots (2)$$

accordingly

$$S^2 = \frac{n}{n-1} s^2 = \frac{1}{n-1} \sum_i (x_i - \bar{x})^2 \quad \dots (3)$$

may be taken as an estimate of σ^2 . The estimated variance of the mean \bar{x} of the sample is thus

$$s'^2 = \frac{S^2}{n} = \frac{1}{n(n-1)} \sum_i (x_i - \bar{x})^2 \quad \dots (4)$$

For large n this is an adequately accurate estimate of the variance of \bar{x} , so that we can easily derive from the sample all that we need for an assessment of the accuracy of the results.

Analogous results hold for multi-dimensional distributions.

2.6.5.2. SHEPPARD'S CORRECTIONS

When n is large it is sometimes convenient to avoid the labour of computing the exact mean and variance of a one-dimensional distribution by *grouping* the data. In this method the range of the variable is divided into a number of intervals of equal length, and each observation is taken to have the value of the mid-point of the interval in which it lies. This simplifies the calculations at the price of a little inaccuracy. On the average the means of the grouped and ungrouped samples are the same, but on the average the variance p^2 of the grouped data is larger than the variance s^2 of the ungrouped data. If h is the length of the intervals the corrected estimate of the sample variance is

$$p^2 - \frac{1}{12} h^2 \quad \dots (5)$$

Corrections of this type, which may be made to any moments of grouped samples, are known as Sheppard's corrections.

2.6.5.3. SMALL SAMPLES

When only a few measurements are made it is no longer possible to appeal to the Central Limit Theorem to decide the distribution of the mean of a sample. In such cases the distribution of the mean can be determined only if the parent distribution $f(x)$ is known. In principle, given $f(x)$, the distribution of the mean can always be calculated by the method described in Section 2.6.2.6 for the distribution of a sum of independent variables.

For certain parent distributions, the distribution of the mean is unusually simple. Thus if $f(x)$ is a normal distribution with mean m and variance σ^2 , the distribution of the sample mean is also normal with the same mean m and variance σ^2/n . If $f(x)$ is a Poisson distribution with parameter λ , the sample mean \bar{x} also has a distribution of the Poisson type with $0, 1/n, 2/n, \dots$ as the possible values of \bar{x} , the probability of $x=a/n$ being $\frac{(n\lambda)^a}{(a!)}e^{-n\lambda}$.

Suppose that we may assume that $f(x)$ is a normal distribution. In assessing the accuracy of the mean \bar{x} of a small sample, we have to allow for the fact that the estimate S^2 of the variance σ^2 of $f(x)$

$$S^2 = \frac{\sum_i (x_i - \bar{x})^2}{n-1} \quad \dots (6)$$

is no longer, as it was with a large sample, a fairly precise estimate of σ^2 . It can be shown that $(n-1)S^2/\sigma^2$ is distributed in a χ^2 distribution (Section 2.6.3.4) with $n-1$ degrees of freedom, and hence that the statistic

$$t = \frac{\bar{x} - m}{s'} \quad \dots (7)$$

where $s' = S/\sqrt{n}$ is the estimate of the standard deviation of \bar{x} , is distributed in Student's distribution (Section 2.6.3.5) with $n-1$ degrees of freedom. As t does not involve the unknown σ it can be used in discussing the accuracy of \bar{x} . The use of t is discussed further in Sections 2.6.6.1 and 2.6.6.2.

2.6.6. Statistical Inference

2.6.6.1. ONE-DIMENSIONAL CONFIDENCE INTERVALS

An experiment may be undertaken either to determine the value of some hitherto unmeasured quantity or to obtain a value for comparison with another estimate of the same or some similar quantity.

In the first case, a typical statement of the results of the experiment will include an estimate of the mean value of the probability distribution of the quantity and an estimate of the accuracy of this determination. It is worth examining in more detail what can be said about the accuracy of the determination. The prin-

ciples involved can be adequately illustrated by supposing that we are considering a mean \bar{x} derived from a small sample of n values, the distribution of the mean being normal.†

Repeated measurements with the same apparatus give no information about the systematic errors of a particular experiment, so that any estimate of the accuracy of \bar{x} derived from the sample values necessarily allows only for the random errors. (The problem of accuracy when a quantity has been measured by several methods is discussed in Section 2.6.6.3.)

The formal knowledge that the mean \bar{x} has variance σ^2/n is of little help in assessing its accuracy, since we do not know σ exactly. However, we can consider the random variable t (Section 2.6.5.3) defined as

$$t = \frac{\bar{x} - m}{s'} \quad \dots (1)$$

where $s' = S/\sqrt{n} = s/\sqrt{(n-1)}$ is the estimated standard deviation of \bar{x} . As has been mentioned, t is distributed in Student's distribution, $s_{n-1}(t)$, with $n-1$ degrees of freedom (Section 2.6.3.5). Since t involves only the unknown m and not the unknown σ^2 , it may be used to discuss the accuracy of \bar{x} as an estimate of m .

The probability that the true mean m lies in the interval $\{\bar{x} + ts', \bar{x} + (t+dt)s'\}$ is $s_{n-1}(t)dt$. [This statement does not imply that the true mean has a probability distribution, for the mean is a fixed, even if unknown, quantity. Whereas usually we speak of the probability of a random variable taking a value in a fixed interval, here we are speaking of the probability of a fixed point being contained in a variable interval, the interval being specified by the sample values \bar{x} and s' .] To specify a range of values within which m is likely to lie we may define *confidence*, or *fiducial*, *ranges* in the following way. For instance, we may define the 99% range as that interval $(\bar{x} + ts', \bar{x} - ts')$ which is such that there is a 99% probability that it includes m . The value of t defining this range satisfies

$$0.99 = \int_{-t}^{+t} s_{n-1}(t) dt \quad \dots (2)$$

The points $\bar{x} + ts'$ and $\bar{x} - ts'$ are then called the 99% *confidence limits*. Confidence ranges for 95%, 99% and 99.9% probabilities for different values of n are readily obtainable from the 5%, 1% and 0.1% values of t_p given in Table 2.6.6A (p. 94).

2.6.6.2. ONE-PARAMETER SIGNIFICANCE TESTS

Suppose alternatively that we wish to compare the experimental mean \bar{x} with a theoretical value ξ_0 , so as to examine whether the theory is supported or opposed by experiment. Again, for simplicity, let us

† The sample mean will be normal if the parent distribution is normal. Whatever the parent distribution, we may also reasonably assume that the sample mean is normal if the sample is sufficiently large (Central Limit Theorem, Sections 2.6.3.3 and 2.6.5.1).

suppose that the distribution of \bar{x} is normal. On the tentative hypothesis that ξ_0 is the true mean m ,

$$t = \frac{\bar{x} - \xi_0}{s'} \quad \dots (3)$$

is a random variable distributed in Student's distribution with $n-1$ degrees of freedom. Let t_0 be the value of t obtained from a particular experiment, and let P be the probability that $|t| \geq |t_0|$. A very small value of P indicates that the occurrence of the results \bar{x} and s' is very surprising if the hypothesis is true, and we may therefore suspect, or even reject, the hypothesis that ξ_0 is the true mean m . On the other hand, if P is not small we conclude that the experimental data are consistent with the hypothesis, though they cannot provide evidence to *prove* that ξ_0 is the *true* value. When P is so small as to cast doubt on the hypothesis we may say that \bar{x} is significantly different from ξ_0 ; just how small P has to be for this is quite arbitrary, and is a compromise between the dangers of falsely rejecting a true hypothesis and of too frequently retaining an incorrect hypothesis. Values of $P=5\%$, 1% and 0.1% are commonly used in testing hypotheses, and are sometimes taken to denote *possibly significant*, *significant* and *highly significant* evidence against a hypothesis. However, it is perhaps wiser to refer to a result as being significant at the 0.1% level rather than as being highly significant. Values of t at the various significance points are given in Table 2.6.6A. The large values of t when the number of degrees of freedom is small should be especially noticed. They reflect the low accuracy of s' as an estimated standard deviation.

In many problems the sample size n exceeds 30, and so to a high degree of approximation the t distribution may be treated as normal. In any case, with large samples our treatment is no longer restricted to normal parent distributions, for we may then reasonably assume that, whatever the parent distribution, the mean \bar{x} is normally distributed. In this case the probability P that $|t| > t_0$ is

$$P = 1 - \left(\frac{2}{\pi}\right)^{\frac{1}{2}} \int_0^{t_0} \exp(-\frac{1}{2}t^2) dt \quad \dots (4)$$

The values of t at the various significance points are then

$P=5\%$	$t=1.960$
$P=1\%$	$t=2.576$
$P=0.1\%$	$t=3.291$
$P=0.01\%$	$t=3.891$

It is possible to compare two experimentally determined mean values and to test the hypothesis that the true means of each quantity are the same. Let the two means be \bar{x}_1 and \bar{x}_2 , with estimated standard deviations s_1' and s_2' . When both samples are large the hypothesis may be tested on the normal law by taking

$$t_0 = \frac{(\bar{x}_1 - \bar{x}_2)}{(s_1'^2 + s_2'^2)^{\frac{1}{2}}} \quad \dots (5)$$

When either or both of the samples are small the distribution of t is more complicated, but the significance points have been tabulated (e.g. Fisher and Yates [73]).

2.6.6.3. WEIGHTED MEAN VALUES AND THE DETECTION OF SYSTEMATIC ERRORS

So far in our discussions of sampling and of statistical inference we have considered only the case in which the sample values were derived by repetitions of the same experiment. Suppose, however, that a quantity is measured by two methods, in one of which the random variable has the distribution $f_a(x)$ and in the other $f_b(x)$. If the means m_a and m_b of the distributions differ, either one or both of the methods is subject to systematic error. On the other hand, if the means coincide it does not imply that both methods are free from systematic error, for the error may be the same in both.

Suppose first that neither method is subject to systematic error. Let \bar{x}_a be the mean of n_a observations by the first method and σ_a^2 be the variance of $f_a(x)$, and let \bar{x}_b , n_b and σ_b^2 be similarly defined. Since both distributions have the same mean, the estimate of lowest variance of this common mean is

$$\bar{\bar{x}} = \left(\frac{n_a}{\sigma_a^2} \bar{x}_a + \frac{n_b}{\sigma_b^2} \bar{x}_b \right) / \left(\frac{n_a}{\sigma_a^2} + \frac{n_b}{\sigma_b^2} \right) \quad \dots (6)$$

the variance of $\bar{\bar{x}}$ is

$$1/(n_a/\sigma_a^2 + n_b/\sigma_b^2) \quad \dots (7)$$

In practice we do not know σ_a and σ_b , and we must replace σ_a^2/n_a and σ_b^2/n_b by the estimated variances $s_a'^2$ and $s_b'^2$ of \bar{x}_a and \bar{x}_b . For large n_a and n_b , whatever $f_a(x)$ and $f_b(x)$, $\bar{\bar{x}}$ will be normally distributed about the true mean with variance $1/(1/s_a'^2 + 1/s_b'^2)$. Confidence ranges and significance levels may be applied as in the earlier case.

Formally, however, we may not assume that the two methods are free from systematic errors. There is no means of telling how far the systematic errors are common to both methods, but we can test whether the systematic errors of the two methods are different by the significance test for the difference of two means which uses t_0 defined by 2.6.6.2(5). If a difference of systematic errors is revealed, we must examine the experimental procedures in an effort to find the causes. Should this search fail, it will be no longer proper to use $\bar{\bar{x}}$ as an estimate of the true value of the quantity, for the discovery of the systematic error implies that the difference $|m_a - m_b|$ is much greater than the standard deviation of the *random* variable $\bar{\bar{x}}$. Further, whether $\bar{\bar{x}}$ is near m_a or m_b is determined by the now irrelevant σ_a , σ_b , n_a and n_b . The wisest course is probably to weight the two methods equally and to take $\frac{1}{2}(\bar{x}_a + \bar{x}_b)$ as an estimate of the true value. The ordinary confidence intervals and significance tests are not applicable to such an estimate.

2.6. STATISTICS

The discussion of accuracy when a quantity is determined by more than two methods will be restricted to the following problem. Suppose a total of n measurements with values x_1, x_2, \dots, x_n is made on a quantity by various methods, the ratios of whose variances, though not the absolute variances, are assumed known. Accordingly the variance of x_i

$$\sigma_i^2 = \sigma^2 / w_i \quad \dots (8)$$

where σ^2 is an unknown constant and the assumed w_i is called the *weight* of the observation x_i . Assuming that there are no systematic errors, the estimate, of lowest variance, of the true mean m is

$$\bar{x} = \frac{w_1 x_1 + \dots + w_n x_n}{w_1 + \dots + w_n} \quad \dots (9)$$

The variance of \bar{x} is

$$\sigma'^2 = \frac{\sigma^2}{w_1 + \dots + w_n} \quad \dots (10)$$

The estimated variance of \bar{x} can be shown to be

$$s'^2 = \frac{\sum w_i (x_i - \bar{x})^2}{\sum w_i} \frac{1}{n-1} \quad \dots (11)$$

and the statistic

$$t = \frac{\bar{x} - m}{s'} \quad \dots (12)$$

has the Student distribution $s_{n-1}(t)$ (Section 2.6.3.5) with $n-1$ degrees of freedom.

If there are systematic errors in the observations s'^2 will be an over-estimate of the variance of the *random* variable \bar{x} (i.e. the spread of the values of \bar{x} obtained in many repetitions of the whole set of measurements will be less than implied by s'^2). Nevertheless, though s'^2 is no longer the estimated variance of a *random* variable, its use through the statistic t will make some allowance for systematic as well as random errors.

Finally, we may illustrate by an example the intimate connection between systematic errors and the true and estimated values of a quantity. Suppose a particular molecular bond length is measured both by the electron diffraction method on the gas and by the X-ray method on a crystal. If the results of the two experiments differ by significantly more than their estimated random errors several explanations are possible: either there is a difference between the bond lengths in the solid and gas phases, or there are unsuspected systematic errors in one or both of the techniques. Further effort must then be directed towards discovering either a reasonable theoretical explanation of the difference in the solid and gas phases or the cause of the unsuspected systematic errors.

2.6.6.4. THE METHOD OF LEAST SQUARES

The *method of least squares* may be used when a number of parameters are to be determined from a larger number of observations. In this method the parameters are chosen to satisfy the criterion that a

weighted sum of the squares of certain *residuals* or *deviations* be a minimum.† The form of the residuals varies from problem to problem. In one case the residuals might be the differences between observed values and values calculated as a function of the parameters. If the best plane through a number of points was being sought, the residuals would be the distances of the points from the plane. Formally, each residual is a function of one or more observations and of one or more parameters.

Let Δ_i be a residual ($i=1, \dots, n$), w_i its weight, and m_r the true value of one of the parameters ($r=1, \dots, k$, and $n > k$). The least squares method consists in choosing estimates u_r of m_r so that

$$R = \sum_{i=1}^n w_i \Delta_i^2 \quad \dots (13)$$

is a minimum.

R is a minimum when

$$\frac{\partial R}{\partial u_r} = 0 \quad (r=1, \dots, k) \quad \dots (14)$$

that is

$$\sum_{i=1}^n w_i \Delta_i \frac{\partial \Delta_i}{\partial u_r} = 0 \quad (r=1, \dots, k) \quad \dots (15)$$

When the Δ_i are linear functions of the u_r , the k conditions (15) are a set of simultaneous linear equations determining the k unknowns u_r . More generally, if the Δ_i are any known functions of the u_r and if an approximate set u_r' of parameters is known, the Δ_i may be expanded to the first order of a multivariate Taylor series. Equation (15) is then linear in the $(u_r - u_r')$.

To save space we will consider only the strictly linear case. We may therefore write

$$\Delta_i = g_i + \sum_{r=1}^k a_{ir} u_r \quad \dots (16)$$

where g_i is independent of the u_r , though possibly a function of one or more observations, and the a_{ir} are either assumed constants or functions of the observations. If Δ_i is not a function of a particular parameter u_r , $a_{ir} = 0$.

$$\text{Accordingly} \quad \frac{\partial \Delta_i}{\partial u_r} = a_{ir} \quad \dots (17)$$

so that the conditions (15) may be written

$$\sum_{s=1}^k b_{rs} u_s = c_r \quad \dots (18)$$

where

$$b_{rs} = \sum_{i=1}^n w_i a_{ir} a_{is} \quad \dots (19a)$$

and

$$c_r = - \sum_{i=1}^n w_i a_{ir} g_i \quad \dots (19b)$$

† When the errors of the observations are normally distributed, the method of least squares leads to the same estimates of the parameters as R. A. Fisher's *maximum likelihood* method.

2.6. STATISTICS

The linear equations (18) are known as the *normal equations*. Their solutions are

$$u_r = \sum_{s=1}^k b^{rs} c_s \quad \dots (20)$$

where b^{rs} is an element of the matrix inverse to (b_{rs}) .

To consider the accuracy of the u_r , suppose first that there are no systematic errors in the observations or in the residuals. For simplicity, suppose further that the residuals, which are random variables when considered as functions of the observations, are each normally distributed and that the weights have been so chosen that

$$w_i = \sigma^2 / \Delta_i^2 \quad \dots (21)$$

where σ^2 is an unknown constant, the same for each residual. It can then be shown that the estimates u_r have a multivariate normal distribution (Section 2.6.4.2) whose mean coincides with the true mean $\mathbf{m} = (m_1, \dots, m_k)$ and whose second order moments are

$$E(u_r - m_r)^2 = b^{rr} \sigma^2 \quad \dots (22a)$$

$$E[(u_r - m_r)(u_s - m_s)] = b^{rs} \sigma^2 \quad \dots (22b)$$

The estimated value of σ^2 is

$$s^2 = \frac{1}{n-k} \sum_i w_i \Delta_i^2 \quad \dots (23)$$

where the Δ_i are calculated with the estimates u_r . $(b^{rr})^{1/2}$ is thus the estimated standard deviation of u_r and the variable

$$t = \frac{u_r - m_r}{(b^{rr})^{1/2} s} \quad \dots (24)$$

has Student's t distribution (Section 2.6.3.5) with $n-k$ degrees of freedom.

If there are systematic errors in the observations or in the residuals (as could occur if insufficient parameters were being employed), $b^{rr} s^2$ will be an overestimate of the variance of the *random* variable u_r (just as s'^2 was of the variance of \bar{x} in Section 2.6.6.3 when there were systematic errors). Nevertheless, though s^2 is no longer the estimated variance of a *random* variable, its use through the statistic t will make some allowance for systematic as well as random errors. In cases where systematic errors are known to be present the weights ought to be chosen to reflect trends in the sizes of the residuals rather than being related to the variances of the residuals considered only as *random* variables.

As an example of the application of the method of least squares in a case where each residual involves one observation and all the parameters, we may mention the application in X-ray crystallography, which is discussed fully in Section 6.4.1.

As an example of a case where each residual involves several observations, we may mention the problem of determining the best plane to pass near a number of points. Here the observations are the three co-ordinates of each point (x_i, y_i, z_i) and the object is

to minimize the weighted sum of the squares of the distances from the plane.

In orthogonal co-ordinates

$$\Delta_i = lx_i + my_i + nz_i - p \quad \dots (25a)$$

and l, m, n and p are the parameters of the plane

$$lx + my + nz - p = 0 \quad \dots (25b)$$

which is to be determined. The parameters are not, however, independent, since $l^2 + m^2 + n^2 = 1$, so that Δ_i is not linear in a set (l, m and p , say) of three independent parameters. Formally, therefore, the normal equations (18) can only be used to determine small changes to an initial approximate set of parameters, whose final values are obtained after several successive applications of the normal equations, as in structure refinement in crystallography.

The general problem in which the points are not nearly coplanar can be more conveniently dealt with by a quite different approach. The best plane must pass through the weighted centre of gravity of the distribution of points. Relative to this origin, the matrix of the weighted second moments

$$\begin{pmatrix} \sum w_i x_i^2 & \sum w_i x_i y_i & \sum w_i x_i z_i \\ \sum w_i x_i y_i & \sum w_i y_i^2 & \sum w_i y_i z_i \\ \sum w_i x_i z_i & \sum w_i y_i z_i & \sum w_i z_i^2 \end{pmatrix} \quad \dots (26)$$

is calculated, and the required direction cosines are then given by the characteristic vector (2.1.8.5, p. 12) with the lowest characteristic value (which is the minimum second moment of the distribution).

If the points are nearly coplanar and if n , say, is known to be the largest direction cosine, the problem can, however, be solved with a single set of normal equations by minimizing the weighted sum $\sum w_i (\Delta z)_i^2$ of the squares of the distances parallel to the z axis from the points to the plane. These distances are

$$(\Delta z)_i = z_i + Lx_i + My_i - P \quad \dots (27)$$

where L, M and P are the parameters to be determined. The normal equations for L, M and P are

$$\begin{cases} b_{xx}L + b_{xy}M + b_xP = c_x \\ b_{xy}L + b_{yy}M + b_yP = c_y \\ b_xL + b_yM + b_0P = c_0 \end{cases} \quad \dots (28a)$$

$$\text{where } \begin{cases} b_{xy} = \sum w_i x_i y_i \\ b_x = -\sum w_i x_i \\ b_0 = \sum w_i \\ c_x = -\sum w_i x_i z_i \\ c_0 = \sum w_i z_i \end{cases} \quad \dots (28b)$$

The required parameters l, m, n and p are then given by $n = (L^2 + M^2 + 1)^{-1/2}$, $l = Ln$, $m = Mn$, $p = Pn$. If the plane is to be constrained to pass through the origin, L and M are determined by omitting the last equation in (28a) and the terms in P in the first two equations. The condition for the equivalence of the minimization of $\sum w_i (\Delta z)_i^2$ with the minimization of the weighted sum of the squares of the orthogonal distances ($\sum w_i \Delta_i^2$) is

that $\sum w_i \Delta_i^2$ should be less than the value of the least significant figure in b_{xx} or b_{yy} .

The method of least squares and the normal equations may also be applied in the fitting of approximations to given functions. An example of this was given in Section 2.2.1.6.1. In such problems, however, the notions of probability are irrelevant.

2.6.6.5. MULTI-PARAMETER CONFIDENCE REGIONS AND SIGNIFICANCE TESTS

When an experiment results in the determination of several parameters, one-parameter significance tests can be applied to each parameter separately, but it may be difficult to interpret the experiment as a whole if some parameters show significant differences and some not. It is therefore preferable to use a test which considers all parameters simultaneously, taking into account their correlations.

Suppose that the experiment provides estimates x_1, x_2, \dots, x_n of n quantities (each corresponding to a mean \bar{x} in the one-parameter case) whose true values are m_1, m_2, \dots, m_n . For simplicity, suppose that the joint probability distribution of x_1, x_2, \dots, x_n is the multivariate normal distribution 2.6.4.2(18).

As with σ^2/n in the one-parameter case, the variance matrix A is unknown, but we can estimate it by methods similar to those used in the one-dimensional case. Let a_{ij} be an element of the estimated variance matrix of the x 's. If the number of measurements in the sample is large, the a_{ij} 's will be adequately accurate estimates. The generalization of the statistic t of Section 2.6.6.1 is the statistic T^2 given by

$$T^2 = \sum_{i=1}^n \sum_{j=1}^n a^{ij} (x_i - m_i)(x_j - m_j) \quad \dots (29)$$

where a^{ij} is an element of the matrix inverse to (a_{ij}) . With large samples, T^2 is distributed as χ^2 with n degrees of freedom (Section 2.6.3.4), and the confidence regions of T^2 are those of χ^2 .

Similarly the hypothesis that the true values of the x 's are $\xi_{01}, \xi_{02}, \dots, \xi_{0n}$ may be tested by calculating

$$T_0^2 = \sum_{i=1}^n \sum_{j=1}^n a_0^{ij} (x_{0i} - \xi_{0i})(x_{0j} - \xi_{0j}) \quad \dots (30)$$

where the x_{0i} are the values obtained in a particular experiment. From the tables of χ^2 (Table 2.6.6B) the probability that $T^2 > T_0^2$ may be found. If this is small, we may reject the hypothesis.

We will mention the distribution of T^2 for small samples only in the case when p parameters have been determined from q independent observations by the method of least squares (as in the determination of X-ray structure parameters, Section 6.4a). Here T^2/p is distributed like F (Section 2.6.3.6), with $m=p$ and $n=q-p$. Tables of the significance points of the F distribution will be found in many statistical texts and tables.

2.6.6.6. χ^2 AS A TEST OF GOODNESS OF FIT

If we make a large number of observations we may use the χ^2 distribution to test the hypothesis that the observations have been sampled from a distribution with probability density $f(x)$.

The range of the variable x is divided into r intervals such that each interval contains at least, say, 10 observations. Let n be the total number of observations, ν_i the number of observations in each interval I_i , and p_i the probability of an observation in the interval I_i if $f(x)$ is the probability density. Then, if the number of observations is large

$$Q = \sum_{i=1}^r \frac{(\nu_i - np_i)^2}{np_i} \quad \dots (31)$$

is distributed like χ^2 (Section 2.6.3.4), with $r-1$ degrees of freedom. The value of Q obtained from the sample values is used to test the hypothesis with the ordinary χ^2 significance test (Table 2.6.6B).

If it is necessary to determine s parameters of $f(x)$ from the sample (say, to estimate the mean and variance of an assumed normal distribution), Q is distributed like χ^2 with $r-s-1$ degrees of freedom.

TABLE 2.6.6A

The Significance Points t_p of the t Distribution

The $P\%$ value t_p is such that the probability of $|t|$ exceeding t_p is $P\%$.

Degrees of Freedom n	t_p as a function of n and P		
	$P=5\%$	$P=1\%$	$P=0.1\%$
1	12.71	63.66	636.62
2	4.30	9.92	31.59
3	3.18	5.84	12.94
4	2.78	4.60	8.61
5	2.57	4.03	6.86
6	2.45	3.71	5.96
7	2.36	3.50	5.40
8	2.31	3.36	5.04
9	2.26	3.25	4.78
10	2.23	3.17	4.59
12	2.18	3.06	4.32
14	2.14	2.98	4.14
16	2.12	2.92	4.02
18	2.10	2.88	3.92
20	2.09	2.84	3.85
30	2.04	2.75	3.65
60	2.00	2.66	3.46
∞	1.96	2.58	3.29

2.6. STATISTICS

TABLE 2.6.6B

The Significance Points χ_p^2 of the χ^2 DistributionThe $P\%$ value χ_p^2 is such that the probability of χ^2 exceeding χ_p^2 is $P\%$.

Degrees of Freedom n	χ_p^2 as a function of n and P				
	$P=99\%$	$P=95\%$	$P=5\%$	$P=1\%$	$P=0.1\%$
1	0.0002	0.004	3.84	6.64	10.83
2	0.020	0.103	5.99	9.21	13.82
3	0.115	0.35	7.82	11.34	16.27
4	0.30	0.71	9.49	13.28	18.47
5	0.55	1.14	11.07	15.09	20.52
6	0.87	1.64	12.59	16.81	22.46
7	1.24	2.17	14.07	18.48	24.32
8	1.65	2.73	15.51	20.09	26.12
9	2.09	3.32	16.92	21.67	27.88
10	2.56	3.94	18.31	23.21	29.59
11	3.05	4.58	19.68	24.72	31.26
12	3.57	5.23	21.03	26.22	32.91
13	4.11	5.89	22.36	27.69	34.53
14	4.66	6.57	23.68	29.14	36.12
15	5.23	7.26	25.00	30.58	37.70
16	5.81	7.96	26.30	32.00	39.25
17	6.41	8.67	27.59	33.41	40.79
18	7.02	9.39	28.87	34.80	42.31
19	7.63	10.12	30.14	36.19	43.82
20	8.26	10.85	31.41	37.57	45.32
21	8.90	11.59	32.67	38.93	46.80
22	9.54	12.34	33.92	40.29	48.27
23	10.20	13.09	35.17	41.64	49.73
24	10.86	13.85	36.42	42.98	51.18
25	11.52	14.61	37.65	44.31	52.62
26	12.20	15.38	38.88	45.64	54.05
27	12.88	16.15	40.11	46.96	55.48
28	13.56	16.93	41.34	48.28	56.89
29	14.26	17.71	42.56	49.59	58.30
30	14.95	18.49	43.77	50.89	59.70

Note: These Tables (2.6.6A and 2.6.6B) are based on R. A. Fisher's *Statistical Methods for Research Workers* (Oliver and Boyd, Edinburgh), 8th Ed., 1941. Acknowledgment is due to the author and to the publishers for permission to use this material.

Section 4 of Volume IV (to be published in 1972) of these International Tables entitled Statistical Significance Tests contains a discussion of the R -factor ratio, and of tests for consistency of weight assignment.

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Section 3

CRYSTAL GEOMETRY

J. D. H. DONNAY AND GABRIELLE DONNAY

	PAGE
3.1. GENERAL RELATIONS, VALID FOR ALL CRYSTAL SYSTEMS	101
3.2. TRICLINIC SYSTEM	106
3.3. MONOCLINIC SYSTEM	107
3.4. ORTHORHOMBIC SYSTEM	108
3.5. TETRAGONAL SYSTEM	109
3.6. HEXAGONAL SYSTEM, <i>sensu lato</i>	112
3.7. RHOMBOHEDRAL SYSTEM, <i>sensu stricto</i>	116
3.8. CUBIC SYSTEM	119
3.9. HEXAGONAL-RHOMBOHEDRAL TRANSFORMATIONS	150

3.1. General Relations, valid for all Crystal Systems

3.1.1. Definition of Terms

Periodicity along m independent directions in n -dimensional space ($m \leq n$):

Triperiodicity ($m=3, n=3$)	Diperiodicity ($m=2, n=2$ or 3)	Monoperiodicity ($m=1, n=1, 2$, or 3)	(No periodicity) ($m=0, n=0, 1, 2$, or 3)
Lattice	Net	Row	Point
<i>Synonyms:</i> Bravais lattice Space lattice 3-dimensional lattice 3-dimensional translation group Translation lattice	Lattice plane Plane lattice 2-dimensional lattice 2-dimensional translation group	Lattice row Line lattice 1-dimensional lattice 1-dimensional translation group	Lattice point Node (French = <i>nœud</i>)

Period in each case:

Cell	Mesh	Parameter	—
<i>Synonyms:</i> Unit cell Elementary parallelepiped	Unit mesh Elementary parallelogram	Repeat distance Interval Translation distance	

The terms *lattice*, *net* and *row* are used to designate periodic assemblages of points. The *net plane* is the plane that contains a net; the *row line* is the line that contains a row. The origin is always taken at a lattice point. Unless otherwise specified, nets and rows are considered to pass through the origin. For short, when there is no danger of confusion, *net* and *row* are used instead of *net plane* and *row line*.

3.1.2. Direct and Reciprocal Lattices

Direct vectors†: a, b, c	Reciprocal vectors†: a*, b*, c*
Reciprocal vectors in terms of direct vectors: $\mathbf{a}^* = \frac{\mathbf{b} \times \mathbf{c}}{\mathbf{a} \cdot \mathbf{b} \times \mathbf{c}}$, etc.	Direct vectors in terms of reciprocal vectors: $\mathbf{a} = \frac{\mathbf{b}^* \times \mathbf{c}^*}{\mathbf{a}^* \cdot \mathbf{b}^* \times \mathbf{c}^*}$, etc.

[where $\mathbf{b} \times \mathbf{c}$ is the vector product of \mathbf{b} and \mathbf{c} , and the dot denotes the scalar product (see Section 2.4.2)] with $\mathbf{a} \cdot \mathbf{b}^* = \mathbf{a} \cdot \mathbf{c}^* = 0$, etc., and $\mathbf{a} \cdot \mathbf{a}^* = 1$, etc.

Volume of cell abc : $V = \mathbf{c} \cdot \mathbf{a} \times \mathbf{b} = \mathbf{a} \cdot \mathbf{b} \times \mathbf{c} = \mathbf{b} \cdot \mathbf{c} \times \mathbf{a}$	Volume of cell a*b*c* : $V^* = \mathbf{c}^* \cdot \mathbf{a}^* \times \mathbf{b}^* = \mathbf{a}^* \cdot \mathbf{b}^* \times \mathbf{c}^* = \mathbf{b}^* \cdot \mathbf{c}^* \times \mathbf{a}^*$
--	---

Relation between Cell Volumes:

$$VV^* = 1$$

This relation holds provided the lattices are primitive (see Vol. I, p. 12, for non-primitive lattices).

3.1.3. The Row Line

The row line‡ [uvw] passes through the origin 000 and the lattice point uvw , where u, v, w are coprime integers.§ The parameter of the row is the length of the lattice vector $\mathbf{L}(uvw)$, which is given by the quadratic form

$$|\mathbf{L}(uvw)|^2 = u^2a^2 + v^2b^2 + w^2c^2 + 2vwbc \cos \alpha + 2wuca \cos \beta + 2uvab \cos \gamma$$

The direction parameters of the row line are the coordinates of the lattice point uvw ; in reciprocal space its direction cosines in terms of the interplanar distance $d(uvw)^*$ are (Fig. 3.1.3):

$$\cos \lambda^* = u \frac{d(uvw)^*}{a^*}, \cos \mu^* = v \frac{d(uvw)^*}{b^*}, \cos \nu^* = w \frac{d(uvw)^*}{c^*}$$

Applications. Parallel to a row in the direct lattice there may be an edge, a zone axis, or a co-ordinate axis; to central rows in the reciprocal lattice correspond face normals and straight lines of reflections on a Weissenberg pattern; and to non-central rows in the reciprocal lattice correspond row lines on a rotation pattern and festoons on a Weissenberg pattern.

† The symbols used are defined in Table 2.4.1, Vol. I, p. 12. K is here taken as 1.

‡ A row line usually needs to be defined in direction only. In the reciprocal lattice, however, it is important to distinguish *non-central row lines*, which do not pass through the origin, from *central row lines*, which do.

§ Integers having no common factor except unity.—Gen. Ed.

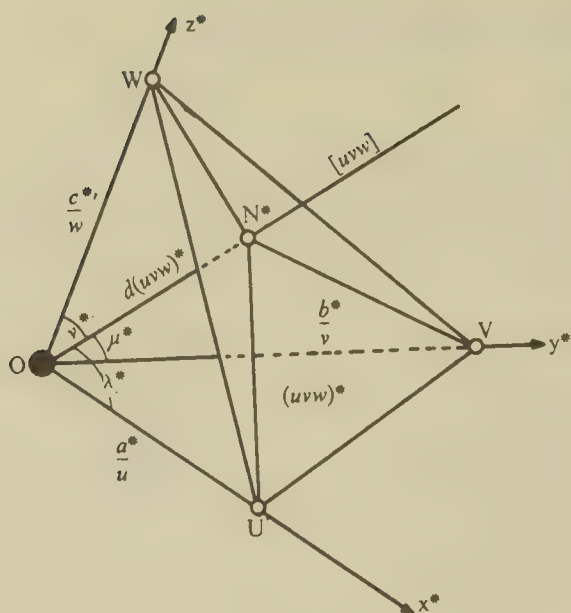


Fig. 3.1.3. Row $[uvw]$ normal to reciprocal net $(uvw)^*$. The black circlet indicates the origin; the empty circlets indicate the intersections of the plane and the lines. They are not necessarily lattice points.

3.1.4. The Net Plane

The net plane† $(hkl)_n$, h, k, l coprime integers‡, has intercepts $n\frac{a}{h}$, $n\frac{b}{k}$, $n\frac{c}{l}$ on the co-ordinate axes. Its equation is

$$h\frac{x}{a} + k\frac{y}{b} + l\frac{z}{c} = n$$

The perpendicular distance between $(hkl)_n$ and $(hkl)_{n+1}$ is the interplanar distance $d(hkl)$. It is inversely proportional to the area $A(hkl)$ of the mesh of the net (hkl) , as $A(hkl) \cdot d(hkl) = V$. Hence $d(hkl) = 1/|L^*(hkl)|$. In direct space the direction cosines of the normal to the net plane (Fig. 3.1.4) are:

$$\cos \lambda = h \frac{d(hkl)}{a}; \cos \mu = k \frac{d(hkl)}{b}; \cos \nu = l \frac{d(hkl)}{c}$$

N.B. If h, k, l are not coprime integers, $(hkl)_1$ is not a net plane.

Applications. Parallel to a net in the direct lattice there may be a crystal face, a cleavage plane, or an X-ray “reflection” plane; to a net in the reciprocal lattice corresponds a plane normal to an edge of the crystal, a layer line on a rotation photograph, a Weissenberg layer or a precession layer.

3.1.5. Fundamental Formula

From the above definition of direction cosines (Fig. 3.1.4) we obtain

$$a:b:c = \frac{h}{\cos \lambda} : \frac{k}{\cos \mu} : \frac{l}{\cos \nu} \quad \dots (1)$$

or

$$h:k:l = a \cos \lambda : b \cos \mu : c \cos \nu \quad \dots (2)$$

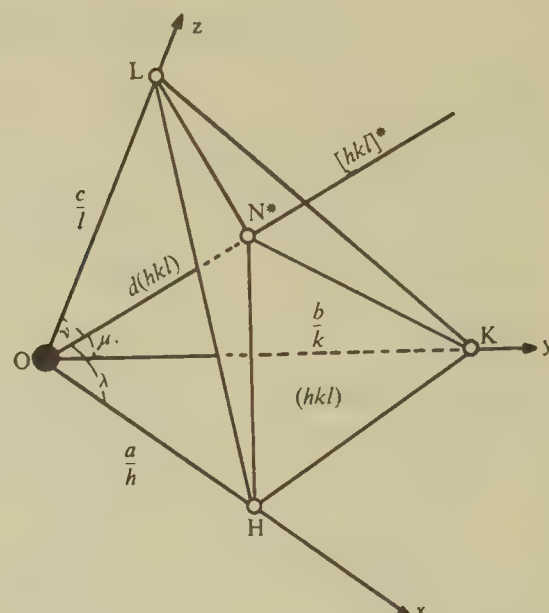


Fig. 3.1.4. Net (hkl) and reciprocal row $[hkl]^*$ normal to it. The black circlet indicates the origin; the empty circlets indicate the intersections of the plane and the lines. They are not necessarily lattice points.

Applications. From the direction angles of the normal to an indexed face (hkl) the axial ratios are obtained by (1). If this face is given the symbol (111) , it is called *unit face* or *parametral face*. Two faces, each parallel to one co-ordinate axis, may be chosen and arbitrarily indexed, instead of a single face that intersects all three axes, e.g. (110) and (011) give respectively $a:b$ and $c:b$.

Once the axial ratios are known, the ratios of the indices for any face (hkl) can be obtained by (2) from the direction cosines of its normal.

3.1.6. Relations between Nets and Rows in One and the Same Space

A net (hkl) contains a row $[uvw]$ if $hu + kv + lw = 0$

Application. A face lying in a zone.

Two nets $(h_1k_1l_1)$ and $(h_2k_2l_2)$ intersect in a row $[uvw]$ if

$$\begin{vmatrix} u & v & w \\ k_1 & l_1 \\ k_2 & l_2 \end{vmatrix} = \begin{vmatrix} u & v & w \\ l_1 & h_1 \\ l_2 & h_2 \end{vmatrix} = \begin{vmatrix} u & v & w \\ h_1 & k_1 \\ h_2 & k_2 \end{vmatrix}$$

Application. A zone axis defined by two faces.

Three nets $(h_1k_1l_1)$, $(h_2k_2l_2)$, $(h_3k_3l_3)$ intersect in a row if

$$\begin{vmatrix} h_1k_1l_1 \\ h_2k_2l_2 \\ h_3k_3l_3 \end{vmatrix} = 0$$

Application. Three faces lying in one zone.

† The subscript is used to designate one particular plane of the family of planes. It indicates the position of this plane with respect to the origin. Thus the plane $(hkl)_0$ is the plane passing through the origin, $(hkl)_n$ the n th plane away from the origin, etc. [1].

‡ Integers having no common factor except unity.—Gen. Ed.

A row $[uvw]$ lies in a net (hkl) if $uh+vk+wl=0$.

Application. A zone containing a face.

Two rows $[u_1v_1w_1]$ and $[u_2v_2w_2]$ lie in a net (hkl) if

$$\begin{vmatrix} h & k & l \\ v_1 & w_1 \\ v_2 & w_2 \end{vmatrix} = \begin{vmatrix} h & k & l \\ w_1 & u_1 \\ w_2 & u_2 \end{vmatrix} = \begin{vmatrix} h & k & l \\ u_1 & v_1 \\ u_2 & v_2 \end{vmatrix}$$

Application. A face belonging to two zones.

Three rows $[u_1v_1w_1]$, $[u_2v_2w_2]$, $[u_3v_3w_3]$ lie in a net if

$$\begin{vmatrix} u_1v_1w_1 \\ u_2v_2w_2 \\ u_3v_3w_3 \end{vmatrix} = 0$$

Application. Three zones having a common face.

Remark. The condition for a line $[uvw]$ to be perpendicular to a plane (hkl) is given for each crystal system under "Twinning" (see also 3.1.9.5, Twin Obliquity).

3.1.7. Relations between Planes in Direct Space and Rows in Reciprocal Space, and vice versa

The family of planes $(nh.nk.nl)$, $n=1, 2, 3, \dots$, in the direct lattice is represented by the lattice point $nh.nk.nl$, $n=1, 2, 3, \dots$, of the row $[hkl]^*$ in the reciprocal lattice. The row is normal to the planes; the length $\sqrt{\{Q(nh.nk.nl)\}}$ of the reciprocal-lattice vector, from the origin to the lattice point $nh.nk.nl$, is equal to $1/d(nh.nk.nl)$. The calculation of d is based on this relation. It is given for each crystal system.

The mesh area $A(hkl)$ of the net (hkl) is equal to $V\sqrt{\{Q(hkl)\}}$.

A net plane $(uvw)_0^*$ containing the origin and lattice points hkl with $uh+vk+wl=0$ of the reciprocal lattice is represented by the row $[uvw]$ in the direct lattice. The row $[uvw]$ is normal to the net plane $(uvw)_0^*$ of the reciprocal lattice. The net planes (hkl) of the direct lattice lie in a zone; $[uvw]$ is their zone axis.

The angle ψ between two direct-lattice rows

$$\psi = [u_1v_1w_1] : [u_2v_2w_2]$$

is given by

$$\tan \psi = \frac{\sqrt{\{\Sigma(v_1w_2 - w_1v_2)^2 a^{*2} + 2\Sigma(w_1u_2 - u_1w_2)(u_1v_2 - v_1u_2)b^*c^* \cos \alpha^*\}}}{V^*[\Sigma u_1u_2a^2 + \Sigma(v_1w_2 + w_1v_2)bc \cos \alpha]}$$

$$\text{or by } \cos \psi = \frac{\Sigma u_1u_2a^2 + \Sigma(v_1w_2 + w_1v_2)bc \cos \alpha}{L(u_1v_1w_1) L(u_2v_2w_2)}$$

where $L(uvw) = \sqrt{(\Sigma u^2a^2 + 2\Sigma vwbc \cos \alpha)}$.

The angle ϕ between two reciprocal-lattice rows is given by similar formulae (see Section 3.2.5).

The angle ω between a direct-lattice row and a reciprocal-lattice row

$$\omega = [uvw] : [hkl]^*$$

is given by

$$\cos \omega = \frac{uh+vk+wl}{L(uvw) L^*(hkl)}$$

where $L^*(hkl) = \sqrt{(\Sigma h^2a^{*2} + 2\Sigma klb^*c^* \cos \alpha^*)}$ (cf. Section 3.1.9.5).

3.1.8. Formulae of Miller

Although given for tautozonal faces, the Miller formulae also hold for coplanar zone axes.

3.1.8.1. DIRECT SINE FORMULA

Consider four tautozonal faces $(h_i k_i l_i)$, where $i=1, 2, 3, 4$, in consecutive order. Let the angle between face normals be ϕ_{ij} . The following relation holds:

$$\frac{\sin \phi_{12} \cdot \sin \phi_{34}}{\sin \phi_{23} \cdot \sin \phi_{14}} = \frac{\begin{vmatrix} h_1 & k_1 \\ h_2 & k_2 \end{vmatrix} \cdot \begin{vmatrix} h_3 & k_3 \\ h_4 & k_4 \end{vmatrix}}{\begin{vmatrix} h_2 & k_2 \\ h_3 & k_3 \end{vmatrix} \cdot \begin{vmatrix} h_1 & k_1 \\ h_4 & k_4 \end{vmatrix}} = \frac{p}{q}$$

in which h and k stand for any two of the three indices h, k, l , provided they do not lead to indeterminacy.

Application. Knowing all the angles and the indices of three of four tautozonal faces, to find the indices of the fourth face.

3.1.8.2. CONVERSE COTANGENT FORMULA

The sine formula can be rewritten as follows [2, 3]:

$$p \cot \phi_{12} + q \cot \phi_{14} = (p+q) \cot \phi_{13}$$

Pardillo [4] has prepared charts† for the graphical determination of angles in crystal zones based on the general formula

$$n \cot 10:mn = m \cot 10:11 + (n-m) \cot 10:01$$

This is the converse cotangent formula given above, written in the Fedorov notation. The correspondence may be seen by writing $p=m$, $q=n-m$, $\phi_{13}=\text{angle } 10:mn$, $\phi_{12}=\text{angle } 10:11$, $\phi_{14}=\text{angle } 10:01$.

Application. Knowing the indices of the four faces and the angles between one face and two of the other three, to find the angle between the first and the fourth faces. For accurate results one of the known angles should be as close to 90° as possible, while the other should not be too close to 0 or 180° .

3.1.8.3. HARMONIC CASE

Four faces are harmonic when a line drawn parallel to one of the face normals, say 1, intersects the others, 2, 3 and 4, in b , c and d , so that $bc=cd$. The indices of face 2 are the sums, and the indices of face 4 the differences, of corresponding indices of faces 3 and 1 (not necessarily coprime): $h_2=nh_3+mh_1, \dots$; $h_4=nh_3-mh_1, \dots$, where m and n are integers, often 1. The cotangent formula then reduces to

$$\cot \phi_{12} + \cot \phi_{14} = 2 \cot \phi_{13}$$

Application. Knowing two of the angles in any harmonic quartet, to find the third one.

† Available through the Spanish National Committee.

3.1.9. Twinning [5]

3.1.9.1. INTRODUCTION

The following treatment is geometrical. The relations given permit the twin operation to be derived from experimental data independently of any theoretical interpretation. Let I and II be two crystals of a twin. They are either congruent or enantiomorphous, so that a rotation will bring II to coincidence either with I or with the enantiomorph of I. In either case, as a lattice (translation group) is always centrosymmetric, the *lattice* of II is congruent to that of I and can be brought to coincide with it by a rotation. There is only one such rotation in the triclinic case, whereas several rotations exist in the other cases.

Let xyz be the co-ordinate axes of I, $x'y'z'$ those of II, chosen so that their positive senses correspond to each other. Any rotation that brings the lattice of II on to the lattice of I brings x' on to x , y' on to y , z' on to z —an operation symbolized $(x'x, y'y, z'z)$ —or brings $x'y'z'$ on to some equivalent octant of the xyz axial cross in the non-triclinic case, for instance $(x'\bar{x}, y'y, z'\bar{z})$. All possible rotations are tabulated under each system.

3.1.9.2. GRAPHICAL DETERMINATION OF ROTATIONS

Plot, on the stereographic net, the poles of the axes xyz and $x'y'z'$. To find the rotation axis T and the rotation angle τ that will bring, for example, $x'y'z'$ on to $\bar{x}y\bar{z}$, draw the great circles that are the perpendicular bisectors of the arcs $x'\bar{x}$, $y'y$, $z'\bar{z}$. They have a common intersection, which is T . The rotation angle τ is given by any one of the three equal angles: $x'T\bar{x}$, $y'Ty$, $z'T\bar{z}$. All possible rotations must be determined before the appropriate rotation or rotations (see below) can be chosen to define the twin law.

3.1.9.3. ANALYTICAL DETERMINATION OF ROTATIONS

From the data calculate the direction cosines of the axes $x'y'z'$ with respect to the axes xyz . Letting uvw be the indices of a straight line in the system xyz , and $u'v'w'$ the indices of the same line in the system $x'y'z'$, we have, if the coordinate system is orthogonal,

$$\begin{aligned} u'a &= ua \cos xx' + vb \cos yx' + wc \cos zx' \\ v'b &= ua \cos xy' + vb \cos yy' + wc \cos zy' \\ w'c &= ua \cos xz' + vb \cos yz' + wc \cos zz' \end{aligned}$$

The rotation axis corresponding to the operation $(x'\bar{y}, y'x, z'z)$, for example, is obtained by letting $u'=\bar{v}$, $v'=u$, $w'=w$ in the above equations and solving for uvw , the indices of T , which need not be integers.

If the coordinate system is not orthogonal, replace the direction cosines in the above equations by the corresponding absolute direction parameters. The absolute direction parameters of a line OP through the origin O are the coordinates of the point P that is at unit distance from O. (Cf. equations (7a) and (2a) in section 2.4.4, page 55.)

The rotation angle τ is obtained from the formulae

$$\sin \frac{\tau}{2} = \frac{\sin \frac{xx'}{2}}{\sin Tx} = \frac{\sin \frac{yy'}{2}}{\sin Ty} = \frac{\sin \frac{zz'}{2}}{\sin Tz}$$

or, if the co-ordinate system xyz is orthogonal, from

$$\cos \tau = \frac{1}{2}(\cos xx' + \cos yy' + \cos zz' - 1)$$

3.1.9.4. CHOICE OF TWIN LAW

Of all the rotations obtained above, at least one is a rotation of 180° , 120° , 90° or 60° about a row, or a rotation of 180° about the normal to a net. In the first case the row is chosen as *twin axis*; in the second case the net is chosen as *twin plane*. (Some authors call the corresponding twins *parallel twin* and *normal twin* respectively.)

When the indices uvw of one of the rotation axes are integers, this axis is twin axis. If uvw are not integers, one must find whether there is a net (hkl) normal to $[uvw]$ by applying the perpendicularity condition (see under the appropriate crystal system). If there is such a net (hkl) , this net is twin plane. If such a net does not exist, that is, if the indices hkl of the plane normal to $[uvw]$ are not integers, the rotation under consideration must be discarded as a possible twin operation.†

3.1.9.5. TWIN OBLIQUITY

The obliquity is the angle ω between the normal to the net (hkl) and the row $[uvw]$ that is quasi-normal to (hkl) , where (hkl) is the twin plane or $[uvw]$ the twin axis.

Let $u'v'w'$ be the indices of the line that is normal to the net (hkl) and $h'k'l'$ the indices of the plane that is normal to the row $[uvw]$. The unprimed indices are integers; the primed indices generally are not. The obliquity ω is given by the following general formula, which simplifies in non-triclinic cases:

$$\cos \omega = \frac{uh + vk + wl}{\sqrt{(uh' + vk' + wl')} \sqrt{(u'h + v'k + w'l)}} \sqrt{\frac{N}{N'}}$$

$$\text{where } N = \frac{a}{h}(au' + bv' \cos \gamma + cw' \cos \beta)$$

$$\text{and } N' = \frac{a}{h'}(au + bv \cos \gamma + cw \cos \beta)$$

or corresponding expressions obtained by cyclic permutations.

The following matrix gives h'/a , k'/b , l'/c as linear combinations of ua , vb , wc :

$$\begin{array}{c|ccc} & ua & vb & wc \\ \hline h'/a & 1 & \cos \gamma & \cos \beta \\ k'/b & \cos \gamma & 1 & \cos \alpha \\ l'/c & \cos \beta & \cos \alpha & 1 \end{array}$$

Its inverse gives $u'a$, $v'b$, $w'c$ in terms of h/a , k/b , l/c :

$$\begin{array}{c|ccc} & h/a & k/b & l/c \\ \hline u'a & \sin^2 \alpha & \cos \alpha \cos \beta - \cos \gamma & \cos \gamma \cos \alpha - \cos \beta \\ v'b & \cos \alpha \cos \beta - \cos \gamma & \sin^2 \beta & \cos \beta \cos \gamma - \cos \alpha \\ w'c & \cos \gamma \cos \alpha - \cos \beta & \cos \beta \cos \gamma - \cos \alpha & \sin^2 \gamma \end{array}$$

(Cf. formula for $\cos \omega$ given in Section 3.1.7.)

† Cases where none of the rotations would lead to a twin operation, as defined here, have been reported in the literature (*Heterozwillinge*, complex twins, etc.). The evidence for their existence is not incontrovertible.

3.1.9.6. TWIN INDEX

The index of the twin is the ratio of the total number of lattice points to the number of lattice points that are restored by twinning. If the index is n , the fraction of lattice points restored by twinning is $1/n$. The restored lattice points, considered by themselves, form the "twin lattice," which pervades the whole edifice but may suffer a slight deviation as it crosses the composition surface. The cell of the twin lattice is either a primitive cell of the crystal lattice, in which case the index of the twin is 1, or a multiple cell of the crystal lattice. This cell, whose symmetry or pseudosymmetry governs the description of the twin, is defined: (1) in the case of a twin axis $[uvw]$, by the parameter of the row that is the twin axis and by the smallest mesh of the net (hkl) that is normal or quasi-normal to it; (2) in the case of a twin plane (hkl) , by the smallest mesh of the net that is the twin plane and by the parameter of the row $[uvw]$ that is normal or quasi-normal

to it. Let V be the volume of the cell of the twin lattice and v that of the smallest cell of the crystal lattice. The index of the twin is V/v or $V/2v$, according as the multiple cell does not carry any lattice point in the centre of its body or in the centre of any of its faces, or does carry such a lattice point. This depends on the mode of centring of the crystal lattice itself. The index of the twin is given for the various possible cases in Table 3.1.9.

Donnay [6] has given examples of twinning calculations where the obliquity is calculated by the formula of Section 3.1.9.5. In any triclinic crystal that has (010) as twin plane the formula of Section 3.1.7 gives the obliquity $\omega = [010]:[010]^*$ as follows:

$$\cos \omega = 1/bb^* = 1/b \frac{ca \sin \beta}{V} = \frac{\Delta}{\sin \beta}$$

$$\text{where } \Delta = \sin \alpha^* \sin \beta \sin \gamma = \sin \alpha \sin \beta^* \sin \gamma \\ = \sin \alpha \sin \beta \sin \gamma^*.$$

TABLE 3.1.9
Twin Index in Terms of $S = |hu + kv + lw|$
Twin plane (hkl) quasi-normal to row $[uvw]$
or twin axis $[uvw]$ quasi-normal to net (hkl)

			Index
The crystal lattice is primitive (P):			
$\begin{cases} S \text{ odd} \\ S \text{ even} \end{cases}$			$\begin{matrix} S \\ S/2 \end{matrix}$
The crystal lattice is one-face-centred (say C):			
$\begin{cases} h+k \text{ odd} \\ h+k \text{ even} \end{cases}$	$\begin{cases} u+v \text{ and } w \text{ not both even} \\ u+v \text{ and } w \text{ both even} \end{cases}$	$\begin{cases} S \text{ odd} \\ S \text{ even} \end{cases}$	$\begin{matrix} S \\ S \\ S/2 \end{matrix}$
		$\begin{cases} S/2 \text{ odd} \\ S/2 \text{ even} \end{cases}$	$\begin{matrix} S/2 \\ S/4 \end{matrix}$
The crystal lattice is body-centred (I):			
$\begin{cases} h+k+l \text{ odd} \\ h+k+l \text{ even} \end{cases}$	$\begin{cases} u, v, w \text{ not all odd} \\ u, v, w \text{ all odd} \end{cases}$	$\begin{cases} S \text{ odd} \\ S \text{ even} \end{cases}$	$\begin{matrix} S \\ S \\ S/2 \end{matrix}$
		$\begin{cases} S/2 \text{ odd} \\ S/2 \text{ even} \end{cases}$	$\begin{matrix} S/2 \\ S/4 \end{matrix}$
The crystal lattice is all-face-centred (F):			
$\begin{cases} u+v+w \text{ odd} \\ u+v+w \text{ even} \end{cases}$	$\begin{cases} h, k, l \text{ not all odd} \\ h, k, l \text{ all odd} \end{cases}$	$\begin{cases} S \text{ odd} \\ S \text{ even} \end{cases}$	$\begin{matrix} S \\ S \\ S/2 \end{matrix}$
		$\begin{cases} S/2 \text{ odd} \\ S/2 \text{ even} \end{cases}$	$\begin{matrix} S/2 \\ S/4 \end{matrix}$

3.2. Triclinic System

3.2.1. Cell†

$$a \neq b \neq c; \alpha \neq \beta \neq \gamma$$

$$V = 2abc \sqrt{\sin s \cdot \sin(s-\alpha) \sin(s-\beta) \cdot \sin(s-\gamma)}$$

where $2s = \alpha + \beta + \gamma$.

3.2.2. Direct Lattice

P ; symmetry $\bar{1}$.

3.2.3. Reciprocal Lattice

$$a^* = \frac{bc \sin \alpha}{V}, b^* = \frac{ca \sin \beta}{V}, c^* = \frac{ab \sin \gamma}{V}$$

$$\cos \alpha^* = \frac{\cos \beta \cos \gamma - \cos \alpha}{\sin \beta \sin \gamma}$$

$$\cos \beta^* = \frac{\cos \gamma \cos \alpha - \cos \beta}{\sin \gamma \sin \alpha}$$

$$\cos \gamma^* = \frac{\cos \alpha \cos \beta - \cos \gamma}{\sin \alpha \sin \beta}$$

$$V^* = a^* b^* c^* \sin \alpha \sin \beta^* \sin \gamma^*$$

$$= a^* b^* c^* \sin \alpha^* \sin \beta \sin \gamma^*$$

$$= a^* b^* c^* \sin \alpha^* \sin \beta^* \sin \gamma$$

3.2.4. Choice of Direct Cell

The usual convention is to use a primitive cell. The Delaunay reduction (Vol. I, p. 530†), applied to any primitive cell, affords the easiest method of arriving at a unique cell [7]. The edges of the reduced cell are the shortest three lattice translations a, b, c that permit α, β, γ to be all $\geq 90^\circ$ and the direction cosines of $[111]$ to be all positive or zero. Uniqueness of setting may be ensured by additional conventions with regard to a, b and c . For determinative purposes the convention $c < a < b$ has been adopted in *Crystal Data* [7], since no symmetry considerations are involved in the triclinic system. In deciding finally on the axes and setting of the unit cell, structural considerations (atomic arrangements, isostructuralism, etc.) have priority.

3.2.5. Interplanar Angle

$\phi = (hkl):(h'k'l')$ in direct lattice, equal to inter-row angle $\phi = [hkl]^*:[h'k'l']^*$ in reciprocal lattice.

$$\cos \phi = \frac{hh'a^*2 + kk'b^*2 + ll'c^*2 + (kl' + lk')b^*c^* \cos \alpha^* + (lh' + hl')c^*a^* \cos \beta^* + (hk' + kh')a^*b^* \cos \gamma^*}{\sqrt{(Q_{hkl} \cdot Q_{h'k'l'})}}$$

(For definition of Q see Section 3.2.6.)

To obtain the inter-row angle $\psi = [uvw]:[u'v'w']$ in the direct lattice, equal to the interplanar angle $\psi = (uvw)^*:(u'v'w')^*$ in the reciprocal lattice, replace in the above formula ϕ by ψ , hkl by uvw , $h'k'l'$ by $u'v'w'$, and starred elements by unstarred elements. This holds for all crystal systems.

3.2.6. Quadratic Form Q and Interplanar Distance d

$$Q_{hkl} = h^2 a^{*2} + k^2 b^{*2} + l^2 c^{*2} + 2klb^*c^* \cos \alpha^* + 2lhc^*a^* \cos \beta^* + 2hka^*b^* \cos \gamma^*$$

$$d_{hkl} = 1/\sqrt{Q_{hkl}}$$

3.2.7. Twinning

3.2.7.1. ONLY ONE POSSIBLE ROTATION

$$(x'x, y'y, z'z)$$

3.2.7.2. PERPENDICULARITY CONDITION

Plane (hkl) perpendicular to line $[uvw]$ if

$$\frac{a}{h}(au + bv \cos \gamma + cw \cos \beta)$$

$$= \frac{b}{k}(au \cos \gamma + bv + cw \cos \alpha)$$

$$= \frac{c}{l}(au \cos \beta + bv \cos \alpha + cw)$$

or if

$$\frac{ua}{\frac{h}{a} \sin^2 \alpha + \frac{k}{b} (\cos \alpha \cos \beta - \cos \gamma) + \frac{l}{c} (\cos \gamma \cos \alpha - \cos \beta)}$$

$$= \frac{vb}{\frac{h}{a} (\cos \alpha \cos \beta - \cos \gamma) + \frac{k}{b} \sin^2 \beta + \frac{l}{c} (\cos \beta \cos \gamma - \cos \alpha)}$$

$$= \frac{wc}{\frac{h}{a} (\cos \gamma \cos \alpha - \cos \beta) + \frac{k}{b} (\cos \beta \cos \gamma - \cos \alpha) + \frac{l}{c} \sin^2 \gamma}$$

No net is necessarily perpendicular to a row.

3.2.7.3. TWINNING CONDITION

The following ratios must approach rational numbers:

$$a^2:b^2:c^2:bc \cos \alpha:ca \cos \beta:ab \cos \gamma$$

† the sign \neq reads "need not be equal to" (see Vol. I, Table 2.3.1, p. 11).

‡ Attention is drawn here to the fact that in some copies of Vol. I, p. 534, the diagrams corresponding to the second and sixth monoclinic reduced cells have been interchanged. The second should have the PQRPTR lettering, the sixth SQUOTO. —Gen. Ed.

3.3. Monoclinic System

3.3.1. Cell†

$$a \neq b \neq c; \alpha = \gamma = 90^\circ; \beta > 90^\circ; V = abc \sin \beta$$

3.3.2. Direct Lattice

Either primitive, *P*, or centred (*C*, *A*, *I*); symmetry $2/m$.

3.3.3. Reciprocal Lattice

$$a^* = 1/a \sin \beta, b^* = 1/b, c^* = 1/c \sin \beta$$

$$\alpha^* = \gamma^* = 90^\circ, \beta^* = 180^\circ - \beta$$

3.3.4. Choice of Direct Cell†

The symmetry direction is called *b*. Two lattice translations (generally the shortest two, in which case $\beta < 120^\circ$) in the net perpendicular to *b* are taken as *c* and *a*.

In order to ensure a unique setting, the angle β between the positive senses of the *c* and *a* axes is generally chosen obtuse and one more convention is necessary: either $c < a$ or $c > a$. The former choice has been adopted in *Crystal Data* for determinative purposes. Either choice may finally be necessary to comply with structural considerations.‡

3.3.5. Interplanar Angle $\phi = (hkl):(h'k'l')$ (cf. 3.2.5)

$$\cos \phi = \frac{hh'a^*{}^2 + kk'b^*{}^2 + ll'c^*{}^2 + (lh' + hl')c^*a^* \cos \beta^*}{\sqrt{(Q_{hkl} \cdot Q_{h'k'l'})}}$$

3.3.6. Quadratic Form *Q* and Interplanar Distance *d*

$$Q_{hkl} = h^2a^*{}^2 + k^2b^*{}^2 + l^2c^*{}^2 + 2lhc^*a^* \cos \beta^*$$

$$d_{hkl} = 1/\sqrt{Q_{hkl}}$$

3.3.7. Twinning

3.3.7.1. TWO POSSIBLE ROTATIONS

$$(x'x, y'y, z'z), (x'\bar{x}, y'y, z'\bar{z})$$

3.3.7.2. PERPENDICULARITY CONDITION

Plane (*hkl*) perpendicular to line [*uvw*] if

$$\frac{a}{h}(au + cw \cos \beta) = \frac{b^2}{k}v = \frac{c}{l}(au \cos \beta + cw)$$

or if

$$ua / \left(\frac{h}{a} - \frac{l}{c} \cos \beta \right) = vb / \frac{k}{b} \sin^2 \beta = wc / \left(\frac{l}{c} - \frac{h}{a} \cos \beta \right)$$

Only one net, (010), is perpendicular to a row, [010].

3.3.7.3. TWINNING CONDITION

The following ratios must approach rational numbers:

$$a^2:b^2:c^2:ca \cos \beta$$

Remark. If only $b^2:c^2:ca \cos \beta$ are near rational numbers, only (*h*0*l*) nets are quasi-perpendicular to rows.

† Standard setting, *b* axis unique (by decision of the Second International Congress of Crystallography, Stockholm, 1951). For special purposes, however, the setting *c* axis unique is permitted (see Vol. I).—Gen. Ed.

‡ If the chosen setting differs from that used for descriptive purposes in Volume I (labelled "Standard" in Vol. I, Table 6.2.1), the data given there for equivalent positions, structure factor formulae, diagrams, etc., cannot be applied without an appropriate transformation.

3.4. Orthorhombic System

3.4.1. Cell

$$a \neq b \neq c; \alpha = \beta = \gamma = 90^\circ; V = abc$$

3.4.2. Direct Lattice

Primitive (*P*); one-face-centred (*C*, *A* or *B*); body-centred (*I*); all-face-centred (*F*); symmetry $2/m2/m2/m$.

3.4.3. Reciprocal Lattice

$$a^* = 1/a, b^* = 1/b, c^* = 1/c$$

$$\alpha^* = \beta^* = \gamma^* = 90^\circ$$

3.4.4. Choice of Direct Cell

The three symmetry directions are taken as cell edges. To ensure uniqueness of setting for determinative purposes they are labelled in *Crystal Data* [7] so that $c < a < b$.

The final choice of setting may be determined by structural considerations.†

3.4.5. Interplanar Angle $\phi = (hkl):(h'k'l')$ (cf. 3.2.5)

$$\cos \phi = \frac{hh'a^{*2} + kk'b^{*2} + ll'c^{*2}}{\sqrt{(Q_{hkl} \cdot Q_{h'k'l'})}}$$

3.4.6. Quadratic Form Q and Interplanar Distance d

$$Q_{hkl} = h^2a^{*2} + k^2b^{*2} + l^2c^{*2}$$

$$d_{hkl} = \frac{abc}{\sqrt{(h^2b^2c^2 + k^2c^2a^2 + l^2a^2b^2)}}$$

3.4.7. Twinning

3.4.7.1. FOUR POSSIBLE ROTATIONS

$x'y'z'$ to coincide with xyz , $x\bar{y}\bar{z}$, $\bar{x}y\bar{z}$, $\bar{x}\bar{y}z$

3.4.7.2. PERPENDICULARITY CONDITION

Plane (hkl) perpendicular to line $[uvw]$ if

$$\frac{a^2}{h}u = \frac{b^2}{k}v = \frac{c^2}{l}w$$

Only three nets are perpendicular to rows, viz. (100), (010), (001) perpendicular to $[100]$, $[010]$, $[001]$ respectively.

3.4.7.3. TWINNING CONDITION

The ratios $a^2:b^2:c^2$ must approach rational numbers. If only one of these ratios is near a rational number, only the nets in the corresponding zone are quasi-perpendicular to rows.

† If the chosen setting differs from that used for descriptive purposes in Vol. I (labelled "Standard" in Vol. I, Table 6.2.1), the data given there for equivalent positions, structure factor formulae, diagrams, etc., cannot be applied without an appropriate transformation.

3.5. Tetragonal System

3.5.1. Cell

$$a=b \neq c; \alpha=\beta=\gamma=90^\circ; V=a^2c$$

3.5.2. Direct Lattice

P (or C), I (or F); symmetry $4/m\ 2/m\ 2/m$

3.5.3. Reciprocal Lattice

$$a^*=b^*=1/a, c^*=1/c$$

$$\alpha^*=\beta^*=\gamma^*=90^\circ$$

3.5.4. Choice of Direct Cell

The smallest cell with full lattice symmetry is chosen: either P (not C) or I (not F).

3.5.5. Interplanar Angle $\phi=(hkl):(h'k'l')$ (cf. 3.2.5)

$$\cos \phi = \frac{(hh' + kk')a^{*2} + ll'c^{*2}}{\sqrt{(Q_{hkl} \cdot Q_{h'k'l'})}}$$

Given a plane $(hk0)$, find the angle $=\phi$ arc tan (h/k) which it makes with (010) (see Table 3.5.5).

3.5.6. Quadratic Form Q and Interplanar Distance d

$$Q_{hkl} = (h^2 + k^2)a^{*2} + l^2c^{*2}$$

$$d_{hkl} = \frac{ac}{\sqrt{\{(h^2 + k^2)c^2 + l^2a^2\}}}$$

Given $h^2 + k^2$, find h and k (see Table 3.5.6).

3.5.7. Twinning

3.5.7.1. EIGHT POSSIBLE ROTATIONS

$x'y'z'$ to coincide with xyz , $x\bar{y}\bar{z}$, $\bar{x}y\bar{z}$, $\bar{x}\bar{y}z$, $\bar{y}xz$, $y\bar{x}z$, yxz , $\bar{y}\bar{x}\bar{z}$.

3.5.7.2. PERPENDICULARITY CONDITION

Plane (hkl) perpendicular to line $[uvw]$ if

$$\frac{a^2}{h}u = \frac{a^2}{k}v = \frac{c^2}{l}w$$

(001) is perpendicular to $[001]$ and $(hk0)$ to $[hk0]$.

3.5.7.3. TWINNING CONDITION

The ratio $c^2:a^2$ must approach a rational number.

TABLE 3.5.5
Interplanar Angles ϕ in the Tetragonal Zone
 $\phi=(010):(hk0)$, with $h < k$

ϕ	Case 1. No condition				Case 2. $(h+k)$ even			
0° 0'	010				020			
5 12	1 11 0				1 11 0			
5 43	1 10 0							
6 20	190				190			
7 8	180							
8 8	170				170			
9 28	160							
11 19	150				150			
12 32	...	290						
14 2	140				...	280		
15 15					3 11 0	
15 57	...	270						
18 26	130				130			
20 33	380					
21 48	...	250			4 10 0
23 12	370		370	
23 58	490				
26 34	120				...	240		
29 3	590
29 45	470				
30 58	350		350	
32 0	580
33 41	...	230			460
35 32	570
36 52	340	
37 52				
38 40	450				
39 48
40 36
45 0	110			670	110			...
								790

3.5. TETRAGONAL SYSTEM

TABLE 3.5.6

Tetragonal Quadratic Forms. Given h^2+k^2 , to find h and k

h^2+k^2	h	k	h^2+k^2	h	k	h^2+k^2	h	k	h^2+k^2	h	k	h^2+k^2	h	k
1	1	0	90	9	3	193	12	7	290	17	1	392	14	14
2	1	1	97	9	4	194	13	5		13	11	394	15	13
4	2	0	98	7	7	196	14	0	292	16	6	397	19	6
5	2	1				197	14	1	293	17	2			
8	2	2	100	10	0				296	14	10	400	20	0
9	3	0		8	6	200	14	2	298	17	3		16	12
			101	10	1		10	10				401	20	1
10	3	1	104	10	2	202	11	9	305	17	4	404	20	2
13	3	2	106	9	5	205	14	3		16	7	405	18	9
16	4	0	109	10	3		13	6	306	15	9	409	20	3
17	4	1				208	12	8						
18	3	3	113	8	7				313	13	12	410	19	7
			116	10	4	212	14	4	314	17	5		17	11
20	4	2	117	9	6	218	13	7	317	14	11	416	20	4
25	5	0												
	4	3	121	11	0	221	14	5	320	16	8	421	15	14
26	5	1	122	11	1		11	10	324	18	0	424	18	10
29	5	2	125	11	2	225	15	0	325	18	1	425	20	5
				10	5		12	9		17	6		19	8
32	4	4	128	8	8	226	15	1		15	10		16	13
34	5	3				229	15	2	328	18	2			
36	6	0	130	11	3							433	17	12
37	6	1		9	7	232	14	6	333	18	3	436	20	6
			136	10	6	233	13	8	337	16	9			
40	6	2	137	11	4	234	15	3	338	17	7	441	21	0
41	5	4								13	13	442	21	1
45	6	3	144	12	0	241	15	4					19	9
49	7	0	145	12	1	242	11	11	340	18	4	445	21	2
				9	8	244	12	10		14	12		18	11
50	7	1	146	11	5	245	14	7	346	15	11	449	20	7
	5	5	148	12	2				349	18	5			
52	6	4	149	10	7	250	15	5				450	21	3
53	7	2					13	9	353	17	8		15	15
58	7	3	153	12	3	256	16	0	356	16	10	452	16	14
			157	11	6	257	16	1				457	21	4
61	6	5							360	18	6	458	17	13
64	8	0	160	12	4	260	16	2	361	19	0			
65	8	1	162	9	9		14	8	362	19	1	461	19	10
	7	4	164	10	8	261	15	6	365	19	2	464	20	8
68	8	2	169	13	0	265	16	3		14	13	466	21	5
				12	5		12	11	369	15	12	468	18	12
72	6	6				269	13	10						
73	8	3	170	13	1				370	19	3	477	21	6
74	7	5		11	7	272	16	4		17	9			
			173	13	2	274	15	7	373	18	7	481	20	9
80	8	4	178	13	3	277	14	9	377	19	4		16	15
81	9	0								16	11	482	19	11
82	9	1	180	12	6	281	16	5				484	22	0
85	9	2	181	10	9	288	12	12	386	19	5	485	22	1
	7	6	185	13	4	289	17	0	388	18	8		17	14
89	8	5		11	8		15	8	389	17	10	488	22	2

3.5. TETRAGONAL SYSTEM

TABLE 3.5.6 (continued)

h^2+k^2	h	k	h^2+k^2	h	k	h^2+k^2	h	k	h^2+k^2	h	k	h^2+k^2	h	k
490	21	7	592	24	4	692	26	4	800	28	4	900	30	0
493	22	3	593	23	8	697	24	11		20	20		24	18
	18	13	596	20	14		21	16	801	24	15	901	30	1
						698	23	13	802	21	19		26	15
500	22	4	601	24	5				808	22	18	904	30	2
	20	10	605	22	11	701	26	5	809	28	5	905	29	8
505	21	8				706	25	9					28	11
	19	12	610	23	9	709	22	15	810	27	9	909	30	3
509	22	5		21	13				818	23	17			
			612	24	6	712	26	6				914	25	17
512	16	16	613	18	17				820	28	6	916	30	4
514	17	15	617	19	16	720	24	12		26	12			
						722	19	19	821	25	14	922	29	9
520	22	6	625	25	0	724	20	18	829	27	10	925	30	5
	18	14		24	7	725	26	7					27	14
521	20	11		20	15		25	10	832	24	16		22	21
522	21	9	626	25	1		23	14	833	28	7	928	28	12
529	23	0	628	22	12	729	27	0				929	23	20
			629	25	2				841	29	0			
530	23	1		23	10	730	27	1		21	20	932	26	16
	19	13					21	17	842	29	1	936	30	6
533	23	2	634	25	3	733	27	2	845	29	2	937	24	19
	22	7	637	21	14	738	27	3		26	13			
538	23	3								22	19	941	29	10
			640	24	8	740	26	8	848	28	8	949	30	7
541	21	10	641	25	4		22	16					25	18
544	20	12	648	18	18	745	27	4	850	29	3			
545	23	4					24	13		27	11	953	28	13
	17	16	650	25	5	746	25	11		25	15	954	27	15
548	22	8		23	11				853	23	18			
549	18	15		19	17	754	27	5	857	29	4	961	31	0
			653	22	13		23	15				962	31	1
554	23	5	656	20	16	757	26	9	865	28	9		29	11
557	19	14	657	24	9					24	17	964	30	8
						761	20	19	866	29	5	965	31	2
562	21	11	661	25	6	765	27	6					26	17
565	23	6	666	21	15		21	18	872	26	14	968	22	22
	22	9				769	25	12	873	27	12			
569	20	13	673	23	12				877	29	6	970	31	3
			674	25	7	772	24	14					23	21
576	24	0	676	26	0	773	22	17	881	25	16	976	24	20
577	24	1		24	10	776	26	10	882	21	21	977	31	4
578	23	7	677	26	1	778	27	7	884	28	10			
	17	17								22	20	980	28	14
			680	26	2	784	28	0				981	30	9
580	24	2		22	14	785	28	1	890	29	7	985	29	12
	18	16	685	26	3		23	16		23	19		27	16
584	22	10		19	18	788	28	2	898	27	13	986	31	5
585	24	3	689	25	8								25	19
	21	12		20	17	793	28	3						
586	19	15					27	8				997	31	6
						794	25	13						
						797	26	11						

3.6. Hexagonal System

(*Sensu lato*, including trigonal)

Hexagonal Axes $xyuz$ and Bravais-Miller 4-index Symbols† $hkil$, with $i=-(h+k)$

3.6.1. Cell

$$a=b \neq c; \alpha=\beta=90^\circ; \gamma=120^\circ; V=abc \sin \gamma.$$

3.6.2. Direct Lattice

P , symmetry $6/m \ 2/m \ 2/m$; or R , symmetry $\bar{3} \ 2/m$.

3.6.3. Reciprocal Lattice

$$a^*=b^*=\frac{2}{a\sqrt{3}}, c^*=\frac{1}{c}; \alpha^*=\beta^*=90^\circ, \gamma^*=60^\circ.$$

† Following usage, the superfluous i is subsequently replaced by a dot.

3.6.4. Choice of Direct Cell

The smallest cell with edges parallel to symmetry directions is chosen. It is always P (not H) or R . If an R -lattice is referred to hexagonal axes, the obverse orientation (Vol. I, p. 20, (a) and (b)) is adopted as standard.

3.6.5. Interplanar Angle $\phi=(hk.l):(h'k'.l')$

$$\cos \phi = \frac{[hh' + kk' + \frac{1}{2}(hk' + kh')]a^{*2} + ll'c^{*2}}{\sqrt{(Q_{hk.l} \cdot Q_{h'k'.l'})}}$$

Given a plane $(hk.0)$, find the angle

$$\phi = \arctan \left(\frac{1}{\sqrt{3}} \frac{h-k}{h+k} \right)$$

which it makes with (11.0) (see Table 3.6.5).

TABLE 3.6.5
Interplanar Angles ϕ in the Hexagonal Zone
 $\phi=(11.0):(hk.0)$, with $h>k$

ϕ	Case 1. No condition						Case 2. $(-h+k)$ divisible by 3					
0° 0'	11.0						11.0					
2 33	76.0						
3 0	65.0							
3 40	54.0								
4 43	43.0									
5 30	75.0							
6 35	...	32.0										96.0
7 35	85.0		85.0	
8 13	53.0									
8 57	74.0			74.0		
9 22	95.0							
10 54	21.0						63.0			
12 31	94.0								
13 0	73.0									
13 54	...	52.0					...	52.0				
14 42	83.0									
16 6	31.0						93.0			
17 16	10 3.0									
17 47	...	72.0										
19 6	41.0						41.0					
20 10	...	92.0										
21 3	51.0											
21 47	...	11 2.0					...	11 2.0				
22 24	61.0											
23 25	71.0						71.0					
24 11	81.0											
24 47	91.0											
25 17	10 1.0						10 1.0					
25 42	11 1.0											
30 0	10.0						30.0					

3.6. HEXAGONAL SYSTEM

TABLE 3.6.6

Hexagonal Quadratic Forms. Given h^2+k^2+hk , to find h and k

h^2+k^2+hk	h	k	h^2+k^2+hk	h	k	h^2+k^2+hk	h	k	h^2+k^2+hk	h	k
1	1	0	111	10	1	237	13	4	361	19	0
3	1	1	112	8	4					16	5
4	2	0	117	9	3	241	15	1	363	11	11
7	2	1				243	9	9	364	18	2
9	3	0	121	11	0	244	10	8		12	10
			124	10	2	247	14	3	367	13	9
12	2	2	127	7	6		11	7			
13	3	1	129	8	5				372	14	8
16	4	0				252	12	6	373	17	4
19	3	2	133	11	1	256	16	0	379	15	7
				9	4	259	15	2			
21	4	1	139	10	3		13	5	381	19	1
25	5	0							387	18	3
27	3	3	144	12	0	268	14	4	388	16	6
28	4	2	147	11	2						
				7	7	271	10	9	397	12	11
31	5	1	148	8	6	273	16	1	399	17	5
36	6	0					11	8		13	10
37	4	3	151	9	5	277	12	7			
39	5	2	156	10	4	279	15	3	400	20	0
			157	12	1				403	19	2
43	6	1				283	13	6		14	9
48	4	4	163	11	3	289	17	0	409	15	8
49	7	0	169	13	0						
	5	3		8	7	291	14	5	412	18	4
						292	16	2	417	16	7
52	6	2	171	9	6						
57	7	1	172	12	2	300	10	10	421	20	1
			175	10	5	301	15	4	427	19	3
61	5	4					11	9		17	6
63	6	3	181	11	4	304	12	8			
64	8	0	183	13	1	307	17	1	432	12	12
67	7	2	189	12	3	309	13	7	433	13	11
									436	14	10
73	8	1	192	8	8	313	16	3	439	18	5
75	5	5	193	9	7	316	14	6			
76	6	4	196	14	0				441	21	0
79	7	3		10	6	324	18	0		15	9
			199	13	2	325	15	5	444	20	2
81	9	0				327	17	2	448	16	8
84	8	2	201	11	5						
			208	12	4	331	11	10	453	19	4
91	6	5				333	12	9	457	17	7
	9	1	211	14	1	336	16	4			
93	7	4	217	13	3	337	13	8	463	21	1
97	8	3		9	8				468	18	6
			219	10	7	343	18	1	469	20	3
100	10	0					14	7		13	12
103	9	2	223	11	6	349	17	3			
108	6	6	225	15	0				471	14	11
109	7	5	228	14	2	351	15	6	475	15	10
			229	12	5						

3.6. HEXAGONAL SYSTEM

TABLE 3.6.6 (continued)

h^2+k^2+hk	h	k	h^2+k^2+hk	h	k	h^2+k^2+hk	h	k	h^2+k^2+hk	h	k
481	19	5	613	19	9	741	25	4	871	29	1
	16	9	619	22	5		20	11		19	15
484	22	0							873	24	9
487	21	2	624	20	8	751	21	10	876	20	14
489	17	8	625	25	0	756	24	6	877	28	3
			628	24	2	757	27	1			
496	20	4							883	21	13
499	18	7	631	15	14	763	26	3	889	27	5
			633	16	13		22	9		25	8
507	22	1	637	23	4	768	16	16			
	13	13		21	7	769	17	15	892	22	12
508	14	12		17	12						
						772	18	14	900	30	0
511	19	6	643	18	11	775	25	5	903	29	2
	15	11				777	23	8		23	11
513	21	3	651	25	1		19	13	907	26	7
516	16	10		19	10						
			652	22	6	784	28	0	912	28	4
523	17	9	657	24	3		20	12	916	24	10
525	20	5				787	27	2	919	18	17
529	23	0	661	20	9						
			669	23	5	793	24	7	921	19	16
532	22	2					21	11	925	20	15
	18	8	673	21	8	796	26	4	927	27	6
			675	15	15						
541	21	4	676	26	0	804	22	10	931	30	1
543	19	7		16	14					25	9
547	14	13	679	25	2	811	25	6		21	14
549	15	12		17	13	813	28	1	937	29	3
						817	23	9	939	22	13
553	23	1	684	18	12		17	16			
	16	11	687	22	7	819	27	3	948	26	8
556	20	6	688	24	4		18	15	949	28	5
559	22	3								23	12
	17	10	691	19	11	823	19	14			
						829	20	13	961	31	0
567	18	9	700	20	10					24	11
			703	26	1	831	26	5	964	30	2
571	21	5		23	6	832	24	8	967	27	7
576	24	0	709	25	3	837	21	12			
577	19	8							972	18	18
579	23	2	711	21	9	841	29	0	973	29	4
						844	28	2		19	17
588	22	4	721	24	5	847	22	11	975	25	10
	14	14		16	15	849	25	7	976	20	16
589	20	7	723	17	14						
	15	13	724	22	8	853	27	4	981	21	15
			727	18	13	859	23	10	988	28	6
592	16	12	729	27	0					22	14
597	17	11				867	17	17			
			732	26	2	868	26	6	991	26	9
601	24	1	733	19	12		18	16	993	31	1
603	21	6	739	23	7				997	23	13
604	18	10							999	30	3
607	23	3									

3.6. HEXAGONAL SYSTEM

3.6.6. Quadratic Form Q and Interplanar Distance d

$$Q_{hk.l} = (h^2 + k^2 + hk)a^{*2} + l^2c^{*2}$$

$$d_{hk.l} = \frac{ac\sqrt{3}}{\sqrt{\{4(h^2 + k^2 + hk)c^2 + 3l^2a^2\}}}$$

Given $h^2 + k^2 + hk$, find h and k (see Table 3.6.6).

3.6.7. Twinning

3.6.7.1. TWELVE POSSIBLE ROTATIONS

$x'y'z'$ to coincide with xyz , $xu\bar{z}$, $\bar{y}\bar{u}z$, $\bar{y}\bar{x}\bar{z}$, uxz , $uy\bar{z}$, $\bar{x}\bar{y}z$, $\bar{x}\bar{u}\bar{z}$, yuz , $yx\bar{z}$, $\bar{u}\bar{x}z$, $\bar{u}\bar{y}\bar{z}$.

3.6.7.2. PERPENDICULARITY CONDITION†

Plane $(hk.l)$ perpendicular to line $[uv0w]$ if

$$\frac{1}{h}\left(u - \frac{v}{2}\right) = \frac{1}{k}\left(v - \frac{u}{2}\right) = \frac{1}{l}w\frac{c^2}{a^2}$$

or if
$$\frac{1}{u}\left(h + \frac{k}{2}\right) = \frac{1}{v}\left(k + \frac{h}{2}\right) = \frac{1}{w}l\frac{3a^2}{4c^2}$$

(00.1) is perpendicular to $[0001]$ and $(hk.0)$ to $[2h+k, h+2k, 0, 0]$.

3.6.7.3. TWINNING CONDITION

The ratio $c^2:a^2$ must approach a rational number.

† The symbol $[uv0w]$ is *not* the Weber 4-index symbol $[UVJW]$, where $U = u - (u+v)/3$, $V = v - (u+v)/3$, $J = -(u+v)/3 = -(U+V)$, $W = w$, [8]. This means that in effect only three of the four hexagonal axes are used for calculations, namely xyz . With the Weber symbolism the perpendicularity condition reads

$$\frac{U}{h} = \frac{V}{k} = \frac{J}{l} = \frac{2}{3} \frac{c^2}{a^2} \frac{W}{l}$$

and $(hki0)$ is perpendicular to $[hki0]$. Note that, in a Weber symbol, the index J is *not* superfluous.

3.7. Rhombohedral System

(*Sensu stricto*, trigonal crystals with rhombohedral lattice)

Rhombohedral Axes and Miller 3-index Symbols

3.7.1. Cell

$$a=b=c; 120^\circ > \alpha = \beta = \gamma \neq 90^\circ;$$

$$V = a^3 \sqrt{1 - 3 \cos^2 \alpha + 2 \cos^3 \alpha}.$$

3.7.2. Direct Lattice

Primitive, but designated R ; symmetry $\bar{3} 2/m$.

3.7.3. Reciprocal Lattice†

$$\cos \frac{\alpha^*}{2} = \frac{1}{2 \cos \frac{\alpha}{2}}; a^* = \frac{1}{a \sin \alpha \sin \alpha^*}$$

3.7.4. Choice of Direct Cell

The smallest rhombohedron is chosen, the lower culminating edges being labelled x_r, y_r, z_r , so as to form a right-handed system (Vol. I, p. 20, (a) and (b)).

3.7.5. Interplanar Angle $\phi = (hkl):(h'k'l')$

$$\cos \phi = \frac{\{hh' + kk' + ll' + [h(k' + l') + k(l' + h') + l(h' + k')] \cos \alpha^*\} a^{*2}}{\sqrt{(Q_{hkl} \cdot Q_{h'k'l'})}}$$

3.7.6. Quadratic Form Q and Interplanar Distance d

$$Q_{hkl} = [(h^2 + k^2 + l^2) + 2(kl + lh + hk) \cos \alpha^*] a^{*2}$$

$$d_{hkl} = 1/\sqrt{Q_{hkl}}$$

Given $h^2 + k^2 + l^2$, find h, k, l and $kl + lh + hk$ (see Table 3.7.6).

3.7.7. Twinning

3.7.7.1. SIX POSSIBLE ROTATIONS

$x'y'z'$ to coincide with $xyz, yzx, zxy, \bar{x}\bar{y}\bar{z}, \bar{y}\bar{z}\bar{x}, \bar{z}\bar{x}\bar{y}$.

3.7.7.2. PERPENDICULARITY CONDITION

Plane (hkl) perpendicular to line $[uvw]$ if

$$\frac{1}{h} [u + (v + w) \cos \alpha] = \frac{1}{k} [v + (w + u) \cos \alpha]$$

$$= \frac{1}{l} [w + (u + v) \cos \alpha]$$

or if

$$\frac{1}{u} [h(1 + \cos \alpha) - (k + l) \cos \alpha]$$

$$= \frac{1}{v} [k(1 + \cos \alpha) - (l + h) \cos \alpha]$$

$$= \frac{1}{w} [l(1 + \cos \alpha) - (h + k) \cos \alpha]$$

(111) is perpendicular to $[111]$ and every net containing the row $[111]$ is perpendicular to a row contained in the net (111).

3.7.7.3. TWINNING CONDITION

$\cos \alpha$ must approach a rational number.

† For alternate formulae cf. Vol. I, Table 2.4.1, p. 13.

3.7. RHOMBOHEDRAL SYSTEM

TABLE 3.7.6

Rhombohedral Quadratic Forms. Given $h^2+k^2+l^2$, to find hkl and $kl+lh+hk$

$h^2+k^2+l^2$	$h\ k\ l$	$kl+lh+hk$			
		$+++$ $---$	$-++$ $+-$	$+-+$ $-+-$	$++-$ $---+$
1	1 0 0	0	0	0	0
2	1 1 0	1	-1	-1	1
3	1 1 1	3	-1	-1	-1
4	2 0 0	0	0	0	0
5	2 1 0	2	-2	-2	2
6	2 1 1	5	-3	-1	-1
8	2 2 0	4	-4	-4	4
9	3 0 0	0	0	0	0
	2 2 1	8	-4	-4	0
10	3 1 0	3	-3	-3	3
11	3 1 1	7	-5	-1	-1
12	2 2 2	12	-4	-4	-4
13	3 2 0	6	-6	-6	6
14	3 2 1	11	-7	-5	1
16	4 0 0	0	0	0	0
17	4 1 0	4	-4	-4	4
	3 2 2	16	-8	-4	-4
18	4 1 1	9	-7	-1	-1
	3 3 0	9	-9	-9	9
19	3 3 1	15	-9	-9	3
20	4 2 0	8	-8	-8	8
21	4 2 1	14	-10	-6	2
22	3 3 2	21	-9	-9	-3
24	4 2 2	20	-12	-4	-4
25	5 0 0	0	0	0	0
	4 3 0	12	-12	-12	12
26	5 1 0	5	-5	-5	5
	4 3 1	19	-13	-11	5
27	5 1 1	11	-9	-1	-1
	3 3 3	27	-9	-9	-9
29	5 2 0	10	-10	-10	10
	4 3 2	26	-14	-10	-2
30	5 2 1	17	-13	-7	3
32	4 4 0	16	-16	-16	16
33	5 2 2	24	-16	-4	-4
	4 4 1	24	-16	-16	8
34	5 3 0	15	-15	-15	15
	4 3 3	33	-15	-9	-9
35	5 3 1	23	-17	-13	7
36	6 0 0	0	0	0	0
	4 4 2	32	-16	-16	0
37	6 1 0	6	-6	-6	6
38	6 1 1	13	-11	-1	-1
	5 3 2	31	-19	-11	-1
40	6 2 0	12	-12	-12	12
41	6 2 1	20	-16	-8	4
	5 4 0	20	-20	-20	20
	4 4 3	40	-16	-16	-8
42	5 4 1	29	-21	-19	11
43	5 3 3	39	-21	-9	-9
44	6 2 2	28	-20	-4	-4
45	6 3 0	18	-18	-18	18
	5 4 2	38	-22	-18	2
46	6 3 1	27	-21	-15	9
48	4 4 4	48	-16	-16	-16
49	7 0 0	0	0	0	0
	6 3 2	36	-24	-12	0
50	7 1 0	7	-7	-7	7
	5 5 0	25	-25	-25	25
	5 4 3	47	-23	-17	-7
51	7 1 1	15	-13	-1	-1
	5 5 1	35	-25	-25	15
52	6 4 0	24	-24	-24	24
53	7 2 0	14	-14	-14	14
	6 4 1	34	-26	-22	14
54	7 2 1	23	-19	-9	5
	6 3 3	45	-27	-9	-9
	5 5 2	45	-25	-25	5

3.7. RHOMBOHEDRAL SYSTEM

TABLE 3.7.6 (continued)

$h^2+k^2+l^2$	h	k	l	$kl+lh+hk$			
				+++	++-	+-+	---
56	6	4	2	44	-28	-20	4
57	7	2	2	32	-24	-4	-4
	5	4	4	56	-24	-16	-16
58	7	3	0	21	-21	-21	21
59	7	3	1	31	-25	-17	11
	5	5	3	55	-25	-25	-5
61	6	5	0	30	-30	-30	30
	6	4	3	54	-30	-18	-6
62	7	3	2	41	-29	-13	1
	6	5	1	41	-31	-29	19
64	8	0	0	0	0	0	0
65	8	1	0	8	-8	-8	8
	7	4	0	28	-28	-28	28
	6	5	2	52	-32	-28	8
66	8	1	1	17	-15	-1	-1
	7	4	1	39	-31	-25	17
	5	5	4	65	-25	-25	-15
67	7	3	3	51	-33	-9	-9
68	8	2	0	16	-16	-16	16
	6	4	4	64	-32	-16	-16
69	8	2	1	26	-22	-10	6
	7	4	2	50	-34	-22	6
70	6	5	3	63	-33	-27	-3
72	8	2	2	36	-28	-4	-4
	6	6	0	36	-36	-36	36
73	8	3	0	24	-24	-24	24
	6	6	1	48	-36	-36	24
74	8	3	1	35	-29	-19	13
	7	5	0	35	-35	-35	35
	7	4	3	61	-37	-19	-5
75	7	5	1	47	-37	-33	23
	5	5	5	75	-25	-25	-25
76	6	6	2	60	-36	-36	12
77	8	3	2	46	-34	-14	2
	6	5	4	74	-34	-26	-14
78	7	5	2	59	-39	-31	11
80	8	4	0	32	-32	-32	32
81	9	0	0	0	0	0	0
	8	4	1	44	-36	-28	20
	7	4	4	72	-40	-16	-16
	6	6	3	72	-36	-36	0
82	9	1	0	9	-9	-9	9
	8	3	3	57	-39	-9	-9
83	9	1	1	19	-17	-1	-1
	7	5	3	71	-41	-29	-1
84	8	4	2	56	-40	-24	8
85	9	2	0	18	-18	-18	18
	7	6	0	42	-42	-42	42
86	9	2	1	29	-25	-11	7
	7	6	1	55	-43	-41	29
	6	5	5	85	-35	-25	-25
88	6	6	4	84	-36	-36	-12
89	9	2	2	40	-32	-4	-4
	8	5	0	40	-40	-40	40
	8	4	3	68	-44	-20	-4
	7	6	2	68	-44	-40	16
90	9	3	0	27	-27	-27	27
	8	5	1	53	-43	-37	27
	7	5	4	83	-43	-27	-13
91	9	3	1	39	-33	-21	15
93	8	5	2	66	-46	-34	14
94	9	3	2	51	-39	-15	3
	7	6	3	81	-45	-39	3
96	8	4	4	80	-48	-16	-16
97	9	4	0	36	-36	-36	36
	6	6	5	96	-36	-36	-24
98	9	4	1	49	-41	-31	23
	8	5	3	79	-49	-31	1
	7	7	0	49	-49	-49	49
99	9	3	3	63	-45	-9	-9
	7	7	1	63	-49	-49	35
	7	5	5	95	-45	-25	-25

3.8. Cubic System

3.8.1. Cell

$$a=b=c, \alpha=\beta=\gamma=90^\circ; V=a^3.$$

3.8.2. Direct Lattice

$$P, I, F; \text{symmetry } 4/m \bar{3} 2/m.$$

3.8.3. Reciprocal Lattice

$$a^*=b^*=c^*=1/a; \alpha^*=\beta^*=\gamma^*=90^\circ.$$

3.8.4. Choice of Direct Cell

The smallest cube is chosen.

3.8.5. Interplanar Angle $\phi=(hkl):(h'k'l')$ (cf. 3.2.5)

Given any plane (hkl) , how many numerically distinct angles does it make with the faces of a given form $\{h'k'l'\}$? The answer to this question is given in Table 3.8.5A. Let the given pole (hkl) be placed at the centre of the stereographic projection. It is sufficient to consider half the poles of $\{h'k'l'\}$, namely those of the upper hemisphere, since this restriction excludes only the obtuse supplementary angles. The number of angles to be expected is given in the last column of Table 3.8.5A; it is equal to one-half the multiplicity of the form $\{h'k'l'\}$. This number, however, is in many cases reduced by symmetry. If the given plane is one of the faces, say $(h'k'l')$, of the given form $\{h'k'l'\}$, one

of the angles becomes zero; this trivial value is omitted from the table.

Given a plane (hkl) , what are the numerically distinct angles which it makes with the other faces of the form to which it belongs and with the faces of other forms? The answer to this question is given in Table 3.8.5B. In it fifteen forms are considered. They are listed in the order of increasing $s=h^2+k^2+l^2$ and include the nine forms with the largest effective interplanar spacings d in each cubic lattice (multiple indices being used when necessary to express the lattice criterion: I , "sum even"; F , "all odd or all even"). The numbers appearing in the rows labelled P, I, F at the head of Table 3.8.5B indicate the order of decreasing d spacings in the appropriate lattice. The list of angles under each form symbol contains as many entries as are required by Table 3.8.5A.

Table 3.8.5B is based on the formula

$$\cos \phi = \frac{hh' + kk' + ll'}{\sqrt{(h^2 + k^2 + l^2)} \sqrt{(h'^2 + k'^2 + l'^2)}}$$

where ϕ is the interplanar angle $(hkl):(h'k'l')$.†

† Table 3.8.5B was constructed with the help of an extended table, compiled by Dr. L. W. McKeehan (private communication), giving angles for the I and F lattices. Additional angles were found in an extension of Bozorth's table [9] submitted by Dr. K. W. Andrews (private communication). Mrs. Beulah Decker computed the remaining angles, checked the whole table, and rearranged it in its present form.

TABLE 3.8.5A

Number of Distinct Interplanar Angles between any Given Plane and all the Faces of a Given Form

Given form Given plane	100	110	111	$hk0$	$h'k'0$ $hk'0$ $h'k0$	hkk	khh	$h'k'k'$ $hk'k'$ $kk'k'$ $h'kk$ $h'hh$	hkl	$h'kl$ $hk'l$ hkl'	$h'k'l'$ $hk'l'$ $h'kl'$ $h'k'l$	Number of angles expected * in hemisphere
100	*1'											3
110	2'	*2'										6
111	1	2'	*1									4
$hk0$	3'	4	2	*6'	8							12
hkk ($h \geq k$)	2	4'	3	6'	6	*5	6	7				12
hkl	3	6	4	12'	12	11	11	12	*16	23'	24	24

Obtuse angles and zero angles are not counted. A primed number means that one of the angles is equal to 90° . The asterisk (*) indicates that the number of expected angles (given in the last column) must be decreased by 1.

3.8. CUBIC SYSTEM

TABLE 3.8.5B
Cubic Interplanar Angles

	100	110	111	210	211	221	310	311	320	321	411	331	332	511	531	
<i>P</i>	1	2	3	4	5	6	7	8	9	10	7	5	9	8	9	
<i>I</i>	2	1	5	8	3		4	4		6						
<i>F</i>	2	3	1	6	7											
100	2 of 90° 0'	2 of 45° 0' 90° 0'	3 of 54° 44'	26° 34' 63° 26' 90° 0'	35° 16' 2 of 65° 54'	2 of 48° 11' 70° 32'	18° 26' 71° 34' 90° 0'	25° 14' 2 of 72° 27'	33° 41' 56° 19' 90° 0'	36° 42' 57° 41' 74° 30'	19° 28' 2 of 76° 22'	2 of 46° 30' 76° 44'	2 of 50° 14' 64° 46'	15° 48' 2 of 78° 54'	32° 19' 59° 32' 80° 16'	100
110	4 of 45° 0' 2 of 90° 0'	4 of 60° 0' 90° 0'	3 of 35° 16' 3 of 90° 0'	18° 26' 2 of 50° 46' 3 of 71° 34'	2 of 30° 0' 54° 44' 2 of 73° 13' 90° 0'	19° 28' 2 of 45° 0' 2 of 76° 22' 90° 0'	26° 34' 2 of 47° 52' 63° 26' 2 of 77° 5'	2 of 31° 29' 3 of 64° 46' 90° 0'	11° 19' 2 of 53° 58' 2 of 66° 54' 78° 41'	19° 6' 40° 54' 55° 28' 67° 48' 2 of 79° 6'	2 of 33° 33' 2 of 60° 0' 70° 32' 90° 0'	13° 16' 2 of 49° 33' 2 of 71° 4' 90° 0'	25° 14' 2 of 41° 5' 2 of 81° 20' 90° 0'	2 of 35° 16' 2 of 57° 1' 74° 12' 90° 0'	17° 1' 44° 11' 2 of 61° 26' 2 of 76° 10'	110
111	4 of 54° 44'	2 of 35° 16' 2 of 90° 0'	3 of 70° 32'	2 of 39° 14' 2 of 75° 2'	19° 28' 2 of 61° 52' 90° 0'	15° 48' 54° 44' 2 of 78° 54'	2 of 43° 5' 2 of 68° 35'	29° 30' 2 of 58° 31' 79° 58'	2 of 36° 49' 2 of 80° 47'	22° 12' 51° 53' 72° 1' 90° 0'	35° 16' 2 of 57° 1' 74° 12'	22° 0' 48° 32' 2 of 82° 23'	10° 2' 60° 30' 2 of 75° 45'	38° 57' 2 of 56° 15' 70° 32'	28° 34' 46° 55' 72° 59' 84° 24'	111
210	4 of 26° 34' 4 of 63° 26' 4 of 90° 0'	2 of 18° 26' 4 of 50° 46' 6 of 71° 34'	6 of 39° 14' 6 of 75° 2'	3 of 36° 52' 53° 8' 4 of 66° 25' 2 of 78° 28' 90° 0'	2 of 24° 6' 2 of 43° 5' 4 of 56° 47' 2 of 79° 29' 2 of 90° 0'	2 of 26° 34' 2 of 41° 49' 2 of 53° 24' 2 of 63° 26' 2 of 72° 39' 2 of 90° 0'	7° 8' 29° 45' 2 of 41° 55' 3 of 60° 15' 2 of 68° 9' 2 of 75° 38' 82° 53'	8° 8' 2 of 31° 57' 2 of 45° 0' 2 of 64° 54' 2 of 73° 34' 3 of 81° 52'	2 of 19° 17' 4 of 47° 36' 2 of 66° 8' 4 of 82° 15'	17° 1' 2 of 33° 13' 3 of 53° 18' 2 of 61° 26' 68° 59' 2 of 83° 8' 90° 0'	2 of 18° 26' 2 of 42° 27' 2 of 50° 46' 2 of 71° 34' 2 of 77° 50' 2 of 83° 57'	2 of 22° 34' 2 of 44° 6' 4 of 59° 8' 2 of 72° 4' 2 of 84° 7'	2 of 30° 54' 2 of 40° 17' 2 of 48° 8' 2 of 67° 35' 2 of 73° 23' 2 of 84° 32'	2 of 18° 47' 2 of 39° 14' 2 of 52° 57' 4 of 75° 2' 2 of 85° 4'	10° 40' 2 of 33° 45' 47° 8' 3 of 58° 3' 2 of 67° 48' 76° 54' 2 of 85° 40'	210
211	4 of 35° 16' 8 of 65° 54'	4 of 30° 0' 2 of 54° 44' 4 of 73° 13' 2 of 90° 0'	3 of 19° 28' 6 of 61° 52' 3 of 90° 0'	2 of 24° 6' 2 of 43° 5' 4 of 56° 47' 2 of 79° 29' 2 of 90° 0'	2 of 33° 33' 2 of 48° 11' 2 of 60° 0' 70° 32' 4 of 80° 24'	2 of 17° 43' 35° 16' 2 of 47° 7' 2 of 65° 54' 3 of 74° 12' 2 of 82° 11'	2 of 25° 4' 2 of 37° 34' 2 of 55° 31' 2 of 63° 4' 4 of 83° 30'	2 of 25° 21' 4 of 49° 48' 2 of 58° 55' 2 of 75° 2' 2 of 82° 35'	2 of 25° 4' 2 of 37° 34' 2 of 55° 31' 2 of 63° 4' 4 of 83° 30'	10° 54' 29° 12' 2 of 40° 12' 49° 6' 56° 56' 77° 24' 83° 44' 90° 0'	15° 48' 2 of 39° 40' 2 of 47° 39' 54° 44' 2 of 61° 14' 2 of 73° 13' 2 of 84° 29'	2 of 20° 31' 3 of 41° 28' 3 of 68° 0' 4 of 79° 12'	2 of 16° 47' 29° 30' 2 of 52° 28' 2 of 64° 12' 2 of 69° 38' 79° 58' 2 of 85° 0'	19° 28' 2 of 38° 13' 3 of 51° 3' 2 of 61° 53' 2 of 71° 41' 2 of 80° 58'	14° 58' 2 of 34° 6' 2 of 46° 22' 56° 30' 2 of 65° 32' 73° 59' 82° 4' 2 of 90° 0'	211
221	8 of 48° 11' 4 of 70° 32'	2 of 19° 28' 4 of 45° 0' 4 of 76° 22' 2 of 90° 0'	3 of 15° 48' 3 of 54° 44' 6 of 78° 54'	2 of 26° 34' 2 of 41° 49' 2 of 53° 24' 2 of 63° 26' 2 of 72° 39' 2 of 90° 0'	2 of 17° 43' 35° 16' 2 of 47° 7' 2 of 65° 54' 3 of 74° 12' 2 of 82° 11'	2 of 27° 16' 38° 57' 4 of 63° 37' 2 of 83° 37' 2 of 90° 0'	2 of 22° 24' 2 of 42° 18' 2 of 49° 40' 2 of 68° 18' 2 of 79° 21' 2 of 84° 42'	2 of 32° 31' 2 of 42° 27' 4 of 58° 12' 2 of 65° 4' 2 of 83° 57'	2 of 22° 24' 2 of 42° 18' 2 of 49° 40' 2 of 68° 18' 2 of 79° 21' 2 of 84° 42'	11° 29' 27° 1' 2 of 36° 42' 2 of 57° 41' 63° 33' 79° 44' 2 of 84° 53'	2 of 30° 12' 2 of 45° 0' 51° 3' 2 of 56° 38' 2 of 66° 52' 2 of 71° 41' 90° 0'	6° 13' 3 of 32° 44' 2 of 57° 38' 2 of 67° 31' 4 of 85° 37'	5° 46' 2 of 22° 30' 44° 43' 2 of 60° 10' 2 of 69° 11' 2 of 81° 50' 2 of 85° 55'	2 of 33° 30' 2 of 45° 7' 3 of 54° 44' 2 of 63° 19' 2 of 71° 17' 86° 19'	16° 42' 2 of 32° 19' 42° 54' 51° 42' 2 of 59° 32' 2 of 73° 38' 2 of 80° 16' 86° 46'	221
310	4 of 18° 26' 4 of 71° 34' 4 of 90° 0'	2 of 26° 34' 4 of 47° 52' 2 of 63° 26' 4 of 77° 5'	6 of 43° 5' 6 of 68° 35'	8° 8' 2 of 31° 57' 2 of 45° 0' 2 of 64° 54' 2 of 73° 34' 3 of 81° 52'	2 of 25° 51' 36° 52' 53° 8' 4 of 72° 33' 2 of 84° 16' 90° 0'	2 of 32° 31' 2 of 42° 27' 4 of 58° 12' 2 of 65° 4' 2 of 83° 57'	15° 15' 3 of 37° 52' 52° 8' 2 of 58° 15' 3 of 74° 45' 2 of 79° 54'	2 of 25° 51' 36° 52' 53° 8' 4 of 72° 33' 2 of 84° 16' 90° 0'	15° 15' 3 of 37° 52' 52° 8' 2 of 58° 15' 3 of 74° 45' 2 of 79° 54'	21° 37' 32° 19' 40° 29' 47° 28' 2 of 53° 44' 59° 32' 2 of 65° 0' 75° 19' 85° 9' 90° 0'	2 of 14° 19' 2 of 34° 56' 2 of 58° 33' 2 of 72° 39' 2 of 81° 26' 2 of 85° 44'	2 of 29° 28' 2 of 43° 29' 2 of 54° 31' 4 of 64° 12' 2 of 90° 0'	2 of 36° 0' 2 of 42° 8' 2 of 52° 39' 2 of 61° 50' 2 of 66° 8' 2 of 78° 20'	2 of 13° 10' 2 of 31° 34' 2 of 60° 52' 2 of 75° 55' 4 of 83° 1'	15° 49' 31° 13' 2 of 41° 33' 50° 6' 57° 41' 2 of 64° 41' 71° 18' 77° 39' 83° 52' 90° 0'	310

3.8. CUBIC SYSTEM

TABLE 3.8.5B (continued)

	100	110	111	210	211	221	310	311	320	321	411	331	332	511	531	
<i>P</i>	1	2	3	4	5	6	7	8	9	10	7	5	9	8	9	
<i>I</i>	2	1	5	8	3		4	4		6						
<i>F</i>	2	3	1	6	7											
311	4 of 25° 14' 8 of 72° 27'	4 of 31° 29' 6 of 64° 46' 2 of 90° 0'	3 of 29° 30' 6 of 58° 31' 3 of 79° 58'	2 of 19° 17' 4 of 47° 36' 2 of 66° 8' 4 of 82° 15'	10° 2' 4 of 42° 24' 3 of 60° 30' 2 of 75° 45' 2 of 90° 0'	2 of 25° 14' 3 of 45° 17' 2 of 59° 50' 4 of 72° 27' 84° 14'	2 of 17° 33' 2 of 40° 17' 2 of 55° 6' 2 of 67° 35' 2 of 79° 0' 2 of 90° 0'	2 of 35° 6' 3 of 50° 29' 2 of 62° 58' 4 of 84° 47'	2 of 23° 6' 2 of 41° 11' 2 of 54° 10' 2 of 65° 17' 2 of 75° 28' 2 of 85° 12'	14° 46' 2 of 36° 19' 3 of 49° 52' 61° 5' 2 of 71° 12' 3 of 80° 44'	5° 46' 2 of 31° 29' 44° 43' 2 of 55° 21' 2 of 64° 46' 2 of 81° 50' 2 of 90° 0'	2 of 25° 57' 2 of 40° 27' 51° 30' 2 of 61° 2' 2 of 69° 46' 3 of 78° 1'	2 of 25° 51' 39° 31' 2 of 50° 0' 2 of 59° 3' 2 of 67° 19' 2 of 75° 6' 90° 0'	9° 27' 2 of 29° 30' 41° 2' 2 of 58° 31' 2 of 66° 2' 2 of 79° 58' 2 of 86° 40'	14° 28' 29° 57' 40° 8' 2 of 48° 30' 2 of 55° 54' 3 of 75° 14' 81° 12' 87° 5'	311
320	4 of 33° 41' 4 of 56° 19' 4 of 90° 0'	2 of 11° 19' 4 of 53° 58' 4 of 66° 54' 2 of 78° 41'	6 of 36° 49' 6 of 80° 47'	7° 8' 29° 45' 2 of 41° 55' 3 of 60° 15' 2 of 68° 9' 2 of 75° 38' 82° 53'	2 of 25° 4' 2 of 37° 34' 2 of 55° 31' 2 of 63° 4' 4 of 83° 30'	2 of 22° 24' 2 of 42° 18' 2 of 49° 40' 2 of 68° 18' 2 of 79° 21' 2 of 84° 42'	15° 15' 3 of 37° 52' 52° 8' 2 of 58° 15' 3 of 74° 45' 2 of 79° 54'	2 of 23° 6' 2 of 41° 11' 2 of 54° 10' 2 of 65° 17' 2 of 75° 28' 2 of 85° 12'	22° 37' 2 of 46° 11' 4 of 62° 31' 67° 23' 2 of 72° 5' 90° 0'	15° 30' 27° 11' 35° 23' 48° 9' 53° 38' 2 of 58° 45' 68° 15' 72° 45' 77° 9' 85° 45' 90° 0'	2 of 23° 46' 2 of 44° 1' 2 of 49° 11' 4 of 70° 55' 2 of 86° 15'	2 of 17° 22' 2 of 45° 35' 2 of 55° 4' 2 of 63° 33' 4 of 79° 0'	2 of 27° 30' 2 of 39° 46' 2 of 44° 48' 2 of 72° 48' 2 of 79° 47' 2 of 90° 0'	2 of 24° 51' 4 of 46° 4' 2 of 68° 4' 2 of 74° 31' 2 of 86° 56'	10° 6' 27° 2' 37° 9' 2 of 52° 27' 58° 57' 2 of 65° 3' 2 of 70° 51' 81° 55' 87° 19'	320
321	8 of 36° 42' 8 of 57° 41' 8 of 74° 30'	4 of 19° 6' 4 of 40° 54' 4 of 55° 28' 4 of 67° 48' 8 of 79° 6'	6 of 22° 12' 6 of 51° 53' 6 of 72° 1' 6 of 90° 0'	2 of 17° 1' 4 of 33° 13' 6 of 53° 18' 4 of 61° 26' 2 of 68° 59' 4 of 83° 8' 2 of 90° 0'	2 of 10° 54' 2 of 29° 12' 4 of 40° 12' 2 of 49° 6' 2 of 56° 56' 6 of 70° 54' 2 of 77° 24' 2 of 83° 44' 2 of 90° 0'	2 of 11° 29' 2 of 27° 1' 4 of 36° 42' 4 of 57° 41' 2 of 63° 33' 4 of 74° 30' 2 of 79° 44' 4 of 84° 53'	2 of 21° 37' 2 of 32° 19' 2 of 40° 29' 2 of 47° 28' 4 of 53° 44' 2 of 59° 32' 4 of 65° 0' 2 of 75° 19' 2 of 85° 9' 2 of 90° 0'	2 of 14° 46' 4 of 36° 19' 6 of 49° 52' 2 of 61° 5' 4 of 71° 12' 6 of 80° 44'	2 of 15° 30' 2 of 27° 11' 2 of 35° 23' 2 of 48° 9' 2 of 53° 38' 4 of 58° 45' 2 of 68° 15' 2 of 72° 45' 2 of 77° 9' 2 of 85° 45' 2 of 90° 0'	2 of 21° 47' 31° 0' 3 of 38° 13' 44° 25' 2 of 50° 0' 2 of 60° 0' 64° 37' 3 of 69° 5' 3 of 73° 24' 81° 47' 4 of 85° 54'	2 of 19° 6' 2 of 35° 1' 2 of 40° 54' 2 of 46° 8' 2 of 50° 57' 4 of 55° 28' 2 of 67° 48' 2 of 71° 38' 2 of 75° 24' 2 of 79° 6' 2 of 86° 23'	2 of 11° 11' 4 of 30° 52' 2 of 42° 38' 2 of 52° 11' 2 of 60° 38' 4 of 68° 25' 4 of 75° 48' 2 of 82° 57' 2 of 90° 0'	2 of 14° 23' 2 of 24° 16' 2 of 31° 16' 2 of 42° 12' 2 of 55° 16' 2 of 59° 3' 2 of 65° 42' 4 of 72° 1' 2 of 78° 8' 2 of 90° 0'	6° 21' 3 of 25° 23' 35° 36' 3 of 43° 43' 2 of 50° 46' 57° 10' 4 of 63° 9' 2 of 68° 49' 74° 16' 2 of 79° 35' 3 of 84° 49' 90° 0'	321	
411	4 of 19° 28' 8 of 76° 22'	4 of 33° 33' 4 of 60° 0' 2 of 70° 32' 2 of 90° 0'	3 of 35° 16' 6 of 57° 1' 3 of 74° 12'	2 of 18° 26' 2 of 42° 27' 2 of 50° 46' 2 of 71° 34' 2 of 77° 50' 2 of 83° 57'	15° 48' 2 of 39° 40' 2 of 47° 39' 54° 44' 2 of 61° 14' 2 of 73° 13' 2 of 84° 29'	2 of 30° 12' 2 of 45° 0' 51° 3' 2 of 56° 38' 2 of 66° 52' 2 of 71° 41' 90° 0'	2 of 14° 19' 2 of 34° 56' 2 of 58° 33' 2 of 72° 39' 2 of 81° 26' 2 of 85° 44'	5° 46' 2 of 31° 29' 44° 43' 2 of 55° 21' 2 of 64° 46' 2 of 81° 50' 2 of 90° 0'	2 of 23° 46' 2 of 44° 1' 2 of 49° 11' 4 of 70° 55' 2 of 86° 15'	19° 6' 35° 1' 40° 54' 46° 8' 50° 57' 2 of 55° 28' 67° 48' 71° 38' 75° 24' 79° 6' 86° 23'	2 of 27° 16' 38° 57' 2 of 60° 0' 2 of 67° 7' 4 of 86° 49'	2 of 30° 6' 2 of 40° 48' 3 of 57° 16' 2 of 64° 22' 2 of 77° 31' 83° 47'	2 of 31° 19' 45° 17' 2 of 49° 13' 2 of 56° 27' 2 of 66° 18' 2 of 69° 24' 84° 14'	3° 40' 2 of 24° 53' 35° 16' 2 of 63° 1' 2 of 68° 43' 2 of 84° 48' 2 of 90° 0'	17° 1' 28° 47' 2 of 44° 11' 2 of 50° 24' 61° 26' 71° 25' 2 of 76° 10' 80° 50' 85° 26'	411

3.8. CUBIC SYSTEM

TABLE 3.8.5B (concluded)

	100	110	111	210	211	221	310	311	320	321	411	331	332	511	531		
P	1	2	3	4	5	6	7	8	9	10	7	5	9	8	9		
I	2	1	5	8	3		4			6							
F	2	3	1	6	7			4									
331	8 of 46° 30' 4 of 76° 44'	2 of 13° 16' 4 of 49° 33' 4 of 71° 4' 2 of 90° 0'	3 of 22° 0' 3 of 48° 32' 6 of 82° 23'	2 of 22° 34' 2 of 44° 6' 4 of 59° 8' 2 of 72° 4' 2 of 84° 7'	2 of 20° 31' 3 of 41° 28' 3 of 68° 0' 4 of 79° 12'	6° 13' 3 of 32° 44' 2 of 57° 38' 2 of 67° 31' 4 of 85° 37'	2 of 29° 28' 2 of 43° 29' 2 of 54° 31' 4 of 64° 12' 2 of 90° 0'	2 of 25° 57' 2 of 40° 27' 51° 30' 2 of 61° 2' 2 of 69° 46' 3 of 78° 1'	2 of 17° 22' 2 of 45° 35' 2 of 55° 4' 2 of 63° 33' 4 of 79° 0'	11° 11' 2 of 30° 52' 42° 38' 52° 11' 60° 38' 2 of 68° 25' 2 of 75° 48' 82° 57' 90° 0'	2 of 30° 6' 2 of 40° 48' 3 of 57° 16' 2 of 64° 22' 2 of 77° 31' 83° 47'	26° 31' 2 of 37° 52' 4 of 61° 44' 2 of 80° 55' 2 of 86° 59'	11° 59' 2 of 28° 18' 38° 30' 2 of 54° 4' 2 of 72° 56' 2 of 84° 23' 2 of 90° 0'	2 of 32° 59' 2 of 41° 22' 2 of 54° 58' 3 of 60° 57' 2 of 77° 15' 87° 28'	14° 12' 26° 53' 35° 29' 48° 46' 2 of 54° 26' 64° 45' 69° 34' 2 of 74° 15' 78° 49' 87° 47'	331	
332	8 of 50° 14' 4 of 64° 46'	2 of 25° 14' 4 of 41° 5' 4 of 81° 20' 2 of 90° 0'	3 of 10° 2' 3 of 60° 30' 6 of 75° 45'	2 of 30° 54' 2 of 40° 17' 2 of 48° 8' 2 of 67° 35' 2 of 73° 23' 2 of 84° 32'	2 of 16° 47' 29° 30' 2 of 52° 28' 2 of 64° 12' 2 of 69° 38' 79° 58' 2 of 85° 0'	5° 46' 2 of 22° 30' 44° 43' 2 of 60° 10' 2 of 69° 11' 2 of 81° 50' 2 of 85° 55'	2 of 36° 0' 2 of 42° 8' 2 of 52° 39' 2 of 61° 50' 2 of 66° 8' 2 of 78° 20'	2 of 25° 51' 39° 31' 2 of 50° 0' 2 of 59° 3' 2 of 67° 19' 2 of 75° 6' 90° 0'	2 of 27° 30' 2 of 39° 46' 2 of 44° 48' 2 of 72° 48' 2 of 79° 47' 2 of 90° 0'	14° 23' 24° 16' 31° 16' 42° 12' 55° 16' 59° 9' 62° 53' 73° 27' 2 of 80° 9' 83° 27' 86° 44'	2 of 31° 19' 45° 17' 2 of 49° 13' 2 of 56° 27' 2 of 66° 18' 2 of 69° 24' 84° 14'	11° 59' 2 of 28° 18' 38° 30' 2 of 54° 4' 2 of 72° 56' 2 of 84° 23' 2 of 90° 0'	2 of 17° 20' 50° 29' 4 of 65° 51' 2 of 79° 31' 2 of 82° 10'	2 of 34° 51' 3 of 48° 58' 2 of 54° 56' 4 of 65° 47' 80° 33'	2 of 32° 59' 2 of 41° 22' 2 of 54° 58' 3 of 60° 57' 2 of 77° 15' 87° 28'	20° 27' 30° 8' 2 of 37° 33' 49° 33' 54° 47' 64° 23' 73° 15' 77° 31' 2 of 81° 43' 85° 52'	332
511	4 of 15° 48' 8 of 78° 54'	4 of 35° 16' 4 of 57° 1' 2 of 74° 12' 2 of 90° 0'	3 of 38° 57' 6 of 56° 15' 3 of 70° 32'	2 of 18° 47' 2 of 39° 14' 2 of 52° 57' 4 of 75° 2' 2 of 85° 4'	19° 28' 2 of 38° 13' 3 of 51° 3' 2 of 61° 53' 2 of 71° 41' 2 of 80° 58'	2 of 33° 30' 2 of 45° 7' 3 of 54° 44' 2 of 63° 19' 2 of 71° 17' 86° 19'	2 of 13° 10' 2 of 31° 34' 2 of 60° 52' 2 of 75° 55' 4 of 83° 1'	9° 27' 2 of 29° 30' 41° 2' 2 of 58° 31' 2 of 66° 2' 2 of 79° 58' 2 of 86° 40'	2 of 24° 51' 4 of 46° 4' 2 of 68° 4' 2 of 74° 31' 2 of 86° 56'	22° 12' 34° 37' 2 of 43° 56' 2 of 51° 53' 59° 3' 65° 42' 2 of 72° 1' 78° 8' 90° 0'	3° 40' 2 of 24° 53' 35° 16' 2 of 63° 1' 2 of 68° 43' 2 of 84° 48' 2 of 90° 0'	2 of 32° 59' 2 of 41° 22' 2 of 54° 58' 3 of 60° 57' 2 of 77° 15' 87° 28'	2 of 34° 51' 3 of 48° 58' 2 of 54° 56' 4 of 65° 47' 80° 33'	2 of 22° 11' 31° 35' 2 of 65° 57' 2 of 70° 32' 4 of 87° 53'	19° 22' 28° 34' 41° 34' 2 of 46° 55' 51° 49' 64° 59' 69° 2' 72° 59' 76° 50' 2 of 84° 24'	511	
531	8 of 32° 19' 8 of 59° 32' 8 of 80° 16'	4 of 17° 1' 4 of 44° 11' 8 of 61° 26' 8 of 76° 10'	6 of 28° 34' 6 of 46° 55' 6 of 72° 59' 6 of 84° 24'	2 of 10° 40' 4 of 33° 45' 2 of 47° 8' 6 of 58° 3' 4 of 67° 48' 2 of 76° 54' 4 of 85° 40'	2 of 14° 58' 4 of 34° 6' 4 of 46° 22' 2 of 56° 30' 4 of 65° 32' 2 of 73° 59' 2 of 82° 4' 4 of 90° 0'	2 of 16° 42' 4 of 32° 19' 2 of 42° 54' 2 of 51° 42' 4 of 59° 32' 4 of 73° 38' 4 of 80° 16' 2 of 86° 46'	2 of 15° 49' 2 of 31° 13' 4 of 41° 33' 2 of 50° 6' 2 of 57° 41' 4 of 64° 41' 2 of 71° 18' 2 of 77° 39' 2 of 83° 52' 2 of 90° 0'	2 of 14° 28' 2 of 29° 57' 2 of 40° 8' 4 of 48° 30' 4 of 55° 54' 6 of 75° 14' 2 of 81° 12' 2 of 87° 5'	2 of 10° 6' 2 of 27° 2' 2 of 37° 9' 4 of 52° 27' 2 of 58° 57' 4 of 65° 3' 4 of 70° 51' 2 of 81° 55' 2 of 87° 19'	6° 21' 3 of 25° 23' 35° 36' 3 of 43° 43' 2 of 50° 46' 57° 10' 4 of 63° 9' 2 of 68° 49' 74° 16' 2 of 79° 35' 3 of 84° 49' 90° 0'	2 of 17° 1' 2 of 28° 47' 4 of 44° 11' 4 of 50° 24' 2 of 61° 26' 2 of 71° 25' 4 of 76° 10' 2 of 80° 50' 2 of 85° 26'	2 of 14° 12' 2 of 26° 53' 2 of 35° 29' 2 of 48° 46' 4 of 54° 26' 2 of 64° 45' 2 of 69° 34' 4 of 74° 15' 2 of 78° 49' 2 of 87° 47'	2 of 20° 27' 2 of 30° 8' 4 of 37° 33' 2 of 49° 33' 2 of 54° 47' 2 of 64° 23' 2 of 73° 15' 2 of 77° 31' 4 of 81° 43' 2 of 85° 52'	19° 28' 2 of 27° 40' 34° 3' 2 of 44° 25' 2 of 48° 55' 2 of 51° 49' 2 of 64° 59' 3 of 60° 56' 64° 37' 2 of 68° 12' 2 of 75° 6' 2 of 78° 28' 3 of 88° 22'	531		

3.8.6. Quadratic Form Q and Interplanar Distance d

$$Q_{hkl} = (h^2 + k^2 + l^2)a^{*2}$$

$$d_{hkl} = a/\sqrt{(h^2 + k^2 + l^2)}$$

Given $h^2 + k^2 + l^2$, find h, k, l . It is useful to consider $s = h^2 + k^2 + l^2$ as a number congruent to $p \pmod{8}$, i.e. $s = 8n + p$, $n = 0, 1, 2, \dots$. Table 3.8.6A is divided into 125 rows, $n = 0$ to 124, and 7 columns, $p = 0$ to 6. The only values which s cannot assume are of the form $4^m \times 7 \pmod{4^m \times 8}$, $m = 0, 1, 2, \dots$ [10]. For $m = 0$ this expression reduces to 7 (mod 8) and column $p = 7$ is accordingly omitted from the table; for $m = 1$ the expression reduces to 28 (mod 32), so that s cannot have values 28, 60, 92, \dots , etc.

The only reflections permitted by the F -lattice are those for which $s = p \pmod{8}$, $p = 0, 3$ and 4. The I -lattice allows reflections for which $s = p \pmod{8}$, p even.

In simple structure types the structure factor expression is the same or varies periodically for reflections whose s values appear in the same column. If observed intensities are recorded in a table arranged like the table of s values, simple structure types can easily be identified [11].

Table 3.8.6A is arranged on two pages facing each other. The values of s will be found on the left-hand page. Below each s value are given \sqrt{s} and mantissa of

$\log s$. The possible (hkl) triplets appear on the right-hand page, near the corresponding s value. An asterisk (*) on an s value indicates that the preceding integer is not equal to the sum of three squares.

Table 3.8.6C lists the reflections permitted by the 17 cubic aspects shown in Table 3.8.6B.† It is used in conjunction with Table 3.8.6A, e.g. for indexing a powder pattern.

3.8.7. Twinning

3.8.7.1. TWENTY-FOUR POSSIBLE ROTATIONS

$x'y'z'$ to coincide with $xyz, x\bar{y}\bar{z}, \bar{x}y\bar{z}, \bar{x}\bar{y}z, zy\bar{x}, xz\bar{y}, yx\bar{z}, \bar{y}\bar{x}\bar{z}, yzx, \bar{y}\bar{z}x, y\bar{z}\bar{x}, \bar{y}z\bar{x}, y\bar{x}z, z\bar{y}x, x\bar{z}y, \bar{x}\bar{z}\bar{y}, zxy, \bar{z}x\bar{y}, \bar{z}\bar{x}y, z\bar{x}\bar{y}, \bar{x}zy, \bar{y}xz, \bar{z}yx, \bar{z}\bar{y}\bar{x}$.

3.8.7.2. PERPENDICULARITY CONDITION

Plane (hkl) perpendicular to line $[uvw]$ if

$$\frac{u}{h} = \frac{v}{k} = \frac{w}{l}$$

Every net (hkl) is perpendicular to a row which has the same indices $[hkl]$.

3.8.7.3. TWINNING CONDITION

None.

† An aspect is a set of systematic absences required by one or by several space groups in a given crystal system (see Vol. I, p. 348, Table 4.4.2).

TABLE 3.8.6A
Cubic Quadratic Forms

$s=h^2+k^2+l^2$, \sqrt{s} and mantissa of $\log s$, for $s=8n+p \neq 4^m \cdot 7 \pmod{4^m \cdot 8}$, $m=0, 1, 2, \dots$

$\begin{matrix} p \\ n \end{matrix}$	0	1	2	3	4	5	6
0	0	1 1.00000 000 000	2 1.41421 301 030	3 1.73205 477 121	4 2.00000 602 060	5 2.23607 698 970	6 2.44949 778 151
1	8 2.82843 903 090	9 3.00000 954 243	10 3.16228 000 000	11 3.31662 041 393	12 3.46410 079 181	13 3.60555 113 943	14 3.74166 146 128
2	16 4.00000 204 120	17 4.12311 230 449	18 4.24264 255 273	19 4.35890 278 754	20 4.47214 301 030	21 4.58258 322 219	22 4.69042 342 423
3	24 4.89898 380 211	25 5.00000 397 940	26 5.09902 414 973	27 5.19615 431 364		29 5.38516 462 398	30 5.47723 477 121
4	32 5.65685 505 150	33 5.74456 518 514	34 5.83095 531 479	35 5.91608 544 068	36 6.00000 556 303	37 6.08276 568 202	38 6.16441 579 784
5	40 6.32456 602 060	41 6.40312 612 784	42 6.48074 623 249	43 6.55744 633 468	44 6.63325 643 453	45 6.70820 653 213	46 6.78233 662 758
6	48 6.92820 681 241	49 7.00000 690 196	50 7.07107 698 970	51 7.14143 707 570	52 7.21110 716 003	53 7.28011 724 276	54 7.34847 732 394
7	56 7.48331 748 188	57 7.54983 755 875	58 7.61577 763 428	59 7.68115 770 852		61 7.81025 785 330	62 7.87401 792 392
8	64 8.00000 806 180	65 8.06226 812 913	66 8.12404 819 544	67 8.18535 826 075	68 8.24621 832 509	69 8.30662 838 849	70 8.36660 845 098
9	72 8.48528 857 332	73 8.54400 863 323	74 8.60233 869 232	75 8.66025 875 061	76 8.71780 880 814	77 8.77496 886 491	78 8.83176 892 095
10	80 8.94427 903 090	81 9.00000 908 485	82 9.05539 913 814	83 9.11043 919 078	84 9.16515 924 279	85 9.21954 929 419	86 9.27362 934 498

TABLE 3.8.6A

An asterisk (*) indicates that the preceding number is not a sum of three squared numbers; a double asterisk signifies the same for the preceding two numbers.

Every s followed by all possible (hkl) triplets

s	$h k l$	s	$h k l$	s	$h k l$	s	$h k l$	s	$h k l$	s	$h k l$
1	1 0 0	50	7 1 0	85	9 2 0	117	10 4 1	146	12 1 1	171	13 1 1
2	1 1 0		5 5 0		7 6 0		9 6 0		11 5 0		11 7 1
3	1 1 1		5 4 3	86	9 2 1		8 7 2		11 4 3		11 5 5
4	2 0 0	51	7 1 1		7 6 1	8	10 3 3		9 8 1		9 9 3
5	2 1 0		5 5 1		6 5 5		9 6 1		9 7 4	2	10 6 6
6	2 1 1	52	6 4 0	88*	6 6 4			7	11 5 1	3	13 2 0
8*	2 2 0	53	7 2 0	89	9 2 2	120*	10 4 2		7 7 7		12 5 2
9	3 0 0		6 4 1		8 5 0	1	11 0 0	8	12 2 0		11 6 4
	2 2 1	54	7 2 1		8 4 3		9 6 2	9	12 2 1		10 8 3
			6 3 3		7 6 2		7 6 6		10 7 0	4	13 2 1
10	3 1 0		5 5 2	90	9 3 0	2	11 1 0		9 8 2		11 7 2
11	3 1 1	56*	6 4 2		8 5 1		9 5 4		8 7 6		10 7 5
12	2 2 2	57	7 2 2		7 5 4		8 7 3			6*	12 4 4
13	3 2 0		5 4 4	91	9 3 1	3	11 1 1	150	11 5 2	7	13 2 2
14	3 2 1	58	7 3 0	93*	8 5 2		7 7 5		10 7 1		8 8 7
16*	4 0 0	59	7 3 1	94	9 3 2	5*	11 2 0		10 5 5	8	13 3 0
17	4 1 0		5 5 3		7 6 3		10 5 0	2*	12 2 2		12 5 3
	3 2 2			96*	8 4 4		10 4 3		10 6 4		9 9 4
18	4 1 1	61*	6 5 0	97	9 4 0		8 6 5	3	12 3 0	9	13 3 1
	3 3 0		6 4 3		6 6 5	6	11 2 1		11 4 4		11 7 3
19	3 3 1	62	7 3 2	98	9 4 1		10 5 1		10 7 2		9 7 7
			6 5 1		8 5 3		9 6 3		9 6 6		
20	4 2 0	64*	8 0 0		7 7 0	8*	8 8 0		8 8 5	180	12 6 0
21	4 2 1	65	8 1 0	99	9 3 3	9	11 2 2	4	12 3 1		10 8 4
22	3 3 2		7 4 0		7 7 1		10 5 2		9 8 3	1	12 6 1
24*	4 2 2		6 5 2		7 5 5		8 8 1	5	11 5 3		10 9 0
25	5 0 0	66	8 1 1	100	10 0 0		8 7 4		9 7 5		9 8 6
	4 3 0		7 4 1		8 6 0			7*	12 3 2	2	13 3 2
26	5 1 0		5 5 4		10 1 0	130	11 3 0		11 6 0		11 6 5
	4 3 1	67	7 3 3	1	9 4 2		9 7 0	8	11 6 1		10 9 1
27	5 1 1	68	8 2 0		8 6 1	1	11 3 1		10 7 3	4*	12 6 2
	3 3 3		6 4 4		7 6 4		9 7 1			5	13 4 0
29*	5 2 0	69	8 2 1	2	10 1 1		9 5 5	160*	12 4 0		12 5 4
	4 3 2		7 4 2		7 7 2	2	10 4 4	1	12 4 1		11 8 0
30	5 2 1	70	6 5 3	4*	10 2 0		8 8 2		11 6 2		10 9 2
32*	4 4 0	72*	8 2 2		8 6 2	3	9 6 4		10 6 5		10 7 6
33	5 2 2		6 6 0	5	10 2 1	4	11 3 2		9 8 4	6	13 4 1
	4 4 1	73	8 3 0		8 5 4		10 5 3	2	12 3 3		11 8 1
34	5 3 0		6 6 1	6	9 5 0		9 7 2		11 5 4		11 7 4
	4 3 3	74	8 3 1		9 4 3	6*	10 6 0		9 9 0	7	13 3 3
35	5 3 1		7 5 0	7	9 5 1		8 6 6		8 7 7		9 9 5
36	6 0 0		7 4 3		7 7 3	7	11 4 0	3	9 9 1	9*	13 4 2
	4 4 2	75	7 5 1		6 6 6		10 6 1	4	12 4 2		12 6 3
37	6 1 0		5 5 5	8	10 2 2		8 8 3		10 8 0		11 8 2
38	6 1 1	76	6 6 2	9	10 3 0		8 8 1		8 8 6		10 8 5
	5 3 2	77	8 3 2		8 6 3	8	11 4 1	5	10 8 1		
40*	6 2 0		6 5 4				8 7 5		10 7 4		
41	6 2 1	78	7 5 2	110	10 3 1	9	11 3 3	6	11 6 3	190	10 9 3
	5 4 0				9 5 2		9 7 3		9 9 2	2*	8 8 8
	4 4 3	80*	8 4 0		7 6 5				9 7 6	3	12 7 0
42	5 4 1	81	9 0 0	3**	10 3 2	140	10 6 2	8*	10 8 2		11 6 6
43	5 3 3		8 4 1		9 4 4	1	11 4 2	9	13 0 0	4	13 5 0
44	6 2 2		7 4 4		8 7 0		10 5 4		12 5 0		13 4 3
45	6 3 0		6 6 3	4	8 7 1	2	9 6 5		12 4 3		12 7 1
	5 4 2	82	9 1 0		8 5 5	4*	12 0 0				12 5 5
46	6 3 1		8 3 3		7 7 4		8 8 4	170	13 1 0		11 8 3
48*	4 4 4	83	9 1 1	5	9 5 3	5	12 1 0		12 5 1		9 8 7
49	7 0 0		7 5 3	6	10 4 0		10 6 3		11 7 0	5	13 5 1
	6 3 2	84	8 4 2		8 6 4		9 8 0		9 8 5		11 7 5

TABLE 3.8.6A (continued)

 $s=h^2+k^2+l^2$, \sqrt{s} and mantissa of $\log s$, for $s=8n+p \neq 4^m \cdot 7 \pmod{4^m \cdot 8}$, $m=0, 1, 2, \dots$

$n \backslash p$	0	1	2	3	4	5	6
11	88 9·38083 944 483	89 9·43398 949 390	90 9·48683 954 243	91 9·53939 959 041		93 9·64365 968 483	94 9·69536 973 128
12	96 9·79796 982 271	97 9·84886 986 772	98 9·89949 991 226	99 9·94987 995 635	100 10·0000 000 000	101 10·0499 004 321	102 10·0995 008 600
13	104 10·1980 017 033	105 10·2470 021 189	106 10·2956 025 306	107 10·3441 029 384	108 10·3923 033 424	109 10·4403 037 426	110 10·4881 041 393
14		113 10·6301 053 078	114 10·6771 056 905	115 10·7238 060 698	116 10·7703 064 458	117 10·8167 068 186	118 10·8628 071 882
15	120 10·9545 079 181	121 11·0000 082 785	122 11·0454 086 360	123 11·0905 089 905		125 11·1803 096 910	126 11·2250 100 371
16	128 11·3137 107 210	129 11·3578 110 590	130 11·4018 113 943	131 11·4455 117 271	132 11·4891 120 574	133 11·5326 123 852	134 11·5758 127 105
17	136 11·6619 133·539	137 11·7047 136 721	138 11·7473 139 879	139 11·7898 143 015	140 11·8322 146 128	141 11·8743 149 219	142 11·9164 152 288
18	144 12·0000 158 362	145 12·0416 161 368	146 12·0830 164 353	147 12·1244 167 317	148 12·1655 170 262	149 12·2066 173 186	150 12·2474 176 091
19	152 12·3288 181 844	153 12·3693 184 691	154 12·4097 187 521	155 12·4499 190 332		157 12·5300 195 900	158 12·5698 198 657
20	160 12·6491 204 120	161 12·6886 206 826	162 12·7279 209 515	163 12·7671 212 188	164 12·8062 214 844	165 12·8452 217 484	166 12·8841 220 108
21	168 12·9615 225 309	169 13·0000 227 887	170 13·0384 230 449	171 13·0767 232 996	172 13·1149 235 528	173 13·1529 238 046	174 13·1909 240 549

TABLE 3.8.6A (continued)

Every s followed by all possible (hkl) triplets

s	h	k	l	s	h	k	l	s	h	k	l	s	h	k	l	s	h	k	l	
196	14	0	0	221*	14	5	0	244	12	10	0	266	16	3	1	289	17	0	0	
	12	6	4		14	4	3		12	8	6		15	5	4		15	8	0	
7	14	1	0		13	6	4	5	15	4	2		13	9	4		12	12	1	
	12	7	2		11	10	0		14	7	0		12	11	1		12	9	8	
	10	9	4		11	8	6		12	10	1		11	9	8					
8	14	1	1	2	14	5	1		10	9	8	7	13	7	7	290	17	1	0	
	13	5	2		13	7	2		14	7	1		11	11	5		16	5	3	
	10	7	7		11	10	1		14	5	5	8	14	6	6		15	8	1	
	9	9	6	4*	12	8	4		11	11	2	9	16	3	2		15	7	4	
				5	15	0	0		11	10	5		14	8	3		13	11	0	
					14	5	2		8*	14	6	4		13	10	0		12	11	5
200*	14	2	0		12	9	0			12	10	2		13	8	6	1	17	1	1
	10	10	0		11	10	2		9	14	7	2		12	11	2		13	11	1
	10	8	6		10	10	5			13	8	4		12	10	5		11	11	7
1	14	2	1	6	15	1	0			11	8	8					2	16	6	0
	13	4	4		12	9	1			10	10	7						12	12	2
	11	8	4		9	9	8						270	15	6	3	3	17	2	0
	10	10	1	7	15	1	1							14	7	5		16	6	1
2	12	7	3		13	7	3		250	15	5	0		13	10	1		15	8	2
	11	9	0		11	9	5			15	4	3		11	10	7		14	9	4
3	13	5	3	8	14	4	4			13	9	0	2*	16	4	0		12	10	7
	11	9	1		10	8	8			12	9	5		12	8	8	4	17	2	1
4	14	2	2	9	15	2	0		1	15	5	1	3	16	4	1		14	7	7
	10	10	2		12	9	2			13	9	1		13	10	2		13	11	2
5	14	3	0		12	7	6			11	11	3	4	16	3	3		13	10	5
	13	6	0							11	9	7		15	7	0	6*	16	6	2
	12	6	5	230	15	2	1			11	9	7		12	11	3		14	10	0
6	14	3	1		14	5	3		3*	12	10	3		12	9	7		14	8	6
	13	6	1		13	6	5		4	15	5	2		15	7	1	7	17	2	2
	11	9	2		11	10	3			14	7	3		15	5	5		16	5	4
	11	7	6		10	9	7			13	9	2		13	9	5		15	6	6
	10	9	5	2*	14	6	0		6*	16	0	0	6	16	4	2		14	10	1
8*	12	8	0	3	15	2	2		7	16	1	0		14	8	4		13	8	8
9	14	3	2		14	6	1			15	4	4	7	15	6	4		12	12	3
	13	6	2		13	8	0			14	6	5		14	9	0	8	17	3	0
	12	8	1		12	8	5			12	8	7		15	7	2		15	8	3
	12	7	4	4	15	3	0			11	10	6		14	9	1	9	17	3	1
	10	10	3		13	8	1		8	16	1	1		13	10	3		15	7	5
	9	8	8		12	9	3			13	8	5		11	11	6		13	11	3
					11	8	7			11	11	4						13	9	7
210	13	5	4	5	15	3	1		9	15	5	3	280*	12	10	6	300	14	10	2
	11	8	5	6	14	6	2			13	9	3	1	16	5	0		10	10	10
1	11	9	3		10	10	6							16	4	3	1	16	6	3
	9	9	7	7	14	5	4							14	9	2		12	11	6
2	14	4	0		13	8	2		260	16	2	0		14	7	6	2	17	3	2
	12	8	2		11	10	4			14	8	0		12	11	4		14	9	5
3	14	4	1	8	15	3	2			12	10	4		10	10	9		11	10	9
	10	8	7		11	9	6		1	16	2	1	2	16	5	1	4*	12	12	4
4	14	3	3							15	6	0		13	8	7		17	4	0
	13	6	3	241**	15	4	0			14	8	1	3	15	7	3		16	7	0
6*	14	4	2		13	6	6			14	7	4		11	9	9		15	8	4
	12	6	6		12	9	4			12	9	6	5*	16	5	2		14	10	3
	10	10	4		15	4	1		2	15	6	1		14	8	5		13	10	6
7	12	8	3		13	8	3			10	9	9		13	10	4	6	17	4	1
	10	9	6		12	7	7		4*	16	2	2		11	10	8		16	7	1
8	13	7	0		11	11	0			14	8	2		15	6	5		16	5	5
	12	7	5		15	3	3			10	10	8	6	14	9	3		15	9	0
	11	9	4	3	13	7	5		5	16	3	0		13	9	6		13	11	4
9	13	7	1		11	11	1			15	6	2	8*	16	4	4		12	9	9
	13	5	5		9	9	9			12	11	0		12	12	0		11	11	8
	11	7	7																	

TABLE 3.8.6A (continued)

 $s=h^2+k^2+l^2$, \sqrt{s} and mantissa of $\log s$, for $s=8n+p \neq 4^m \cdot 7 \pmod{4^m \cdot 8}$, $m=0, 1, 2, \dots$

$\begin{array}{c} p \\ n \end{array}$	0	1	2	3	4	5	6
22	176 13·2665 245 513	177 13·3041 247 973	178 13·3417 250 420	179 13·3791 252 853	180 13·4164 255 273	181 13·4536 257 679	182 13·4907 260 071
23	184 13·5647 264 818	185 13·6015 267 172	186 13·6382 269 513	187 13·6748 271 842		189 13·7477 276 462	190 13·7840 278 754
24	192 13·8564 283 301	193 13·8924 285 557	194 13·9284 287 802	195 13·9642 290 035	196 14·0000 292 256	197 14·0357 294 466	198 14·0712 296 665
25	200 14·1421 301 030	201 14·1774 303 196	202 14·2127 305 351	203 14·2478 307 496	204 14·2829 309 630	205 14·3178 311 754	206 14·3527 313 867
26	208 14·4222 318 063	209 14·4568 320 146	210 14·4914 322 219	211 14·5258 324 282	212 14·5602 326 336	213 14·5945 328 380	214 14·6287 330 414
27	216 14·6969 334 454	217 14·7309 336 460	218 14·7648 338 456	219 14·7986 340 444		221 14·8661 344 392	222 14·8997 346 353
28	224 14·9666 350 248	225 15·0000 352 183	226 15·0333 354 108	227 15·0665 356 026	228 15·0997 357 935	229 15·1327 359 835	230 15·1658 361 728
29	232 15·2315 365 488	233 15·2643 367 356	234 15·2971 369 216	235 15·3297 371 068	236 15·3623 372 912	237 15·3948 374 748	238 15·4272 376 577
30		241 15·5242 382 017	242 15·5563 383 815	243 15·5885 385 606	244 15·6205 387 390	245 15·6525 389 166	246 15·6844 390 935
31	248 15·7480 394 452	249 15·7797 396 199	250 15·8114 397 940	251 15·8430 399 674		253 15·9060 403 121	254 15·9374 404 834
32	256 16·0000 408 240	257 16·0312 409 933	258 16·0624 411 620	259 16·0935 413 300	260 16·1245 414 973	261 16·1555 416 641	262 15·1864 418 301

TABLE 3.8.6A (continued)

Every s followed by all possible (hkl) triplets

<i>s</i>	<i>h</i>	<i>k</i>	<i>l</i>	<i>s</i>	<i>h</i>	<i>k</i>	<i>l</i>	<i>s</i>	<i>h</i>	<i>k</i>	<i>l</i>	<i>s</i>	<i>h</i>	<i>k</i>	<i>l</i>	<i>s</i>	<i>h</i>	<i>k</i>	<i>l</i>	
307	17	3	3	329	18	2	1	349*	18	5	0	369**	19	2	2	387	19	5	1	
	15	9	1		17	6	2		18	4	3		18	6	3		17	7	7	
8	16	6	4		16	8	3		14	12	3		17	8	4		15	9	9	
	12	10	8		15	10	2		13	12	6		16	8	7		13	13	7	
9	17	4	2		13	12	4						15	12	0	8	18	8	0	
	16	7	2		12	11	8						14	13	2		12	12	10	
	14	8	7										13	10	10	9	18	8	1	
								350	18	5	1		12	12	9		18	7	4	
									17	6	5						17	10	0	
310	15	9	2	330	17	5	4		15	11	2						17	8	6	
	15	7	6		16	7	5		15	10	5						15	10	8	
2*	14	10	4	1	15	9	5		13	10	9	370	19	3	0		14	12	7	
3	14	9	6		13	9	9		12	12	8		17	9	0					
	13	12	0	2	18	2	2	2*	18	5	2		15	12	1					
	12	12	5		14	10	6	3	17	8	0		15	9	8					
4	17	5	0	3	18	3	0		16	9	4	1	19	3	1	390	19	5	2	
	17	4	3		14	11	4		15	8	8		17	9	1		17	10	1	
	16	7	3		13	10	8		14	11	6		15	11	5		14	13	5	
	15	8	5	4	18	3	1	4	17	8	1		13	11	9	2*	18	8	2	
	13	12	1		17	6	3		17	7	4	2	16	10	4		16	10	6	
	13	9	8	6*	16	8	4		16	7	7	3	18	7	0		14	14	0	
	12	11	7	7	18	3	2		13	13	4		16	9	6	3	19	4	4	
5	17	5	1		16	9	0	5	13	11	8	4	15	12	2		17	10	2	
	15	9	3		12	12	7		15	11	3		18	7	1		16	11	4	
	13	11	5	8	17	7	0	6	15	9	7		18	5	5		14	14	1	
7*	16	6	5		16	9	1		16	10	0		17	9	2	4	15	13	0	
	14	11	0		15	8	7		16	8	6		17	7	6		15	12	5	
	13	12	2		13	13	0		14	12	4		15	10	7		13	12	9	
8	17	5	2		13	12	5	7	17	8	2		14	13	3	5	19	5	3	
	14	11	1	9	17	7	1		16	10	1	6*	13	13	6		17	9	5	
	13	10	7		17	5	5		18	5	3		18	6	4		15	13	1	
					13	13	1		14	9	9		14	12	6		15	11	7	
					13	11	7					7	19	4	0	6	18	6	6	
													18	7	2		14	14	2	
320*	16	8	0										16	11	0		14	10	10	
1	17	4	4										14	10	9	7	19	6	0	
	16	8	1										13	12	8		18	8	3	
	16	7	4	340	18	4	0		360*	18	6	0	8	19	4	1	8	19	6	1
	14	11	2		14	12	0			16	10	2		17	8	5		18	7	5
	14	10	5	1	18	4	1		1	19	0	0		16	11	1		17	10	3
	11	10	10		17	6	4			18	6	1		15	12	3		15	13	2
2	15	9	4		16	9	2			17	6	6		19	3	3		14	11	9
	13	12	3		16	7	6			15	10	6		17	9	3				
3	17	5	3		15	10	4		2	19	1	0								
	15	7	7		14	12	1			17	8	3								
	11	11	9		14	9	8			16	9	5								
4	18	0	0	2	18	3	3			15	11	4	381*	19	4	2	400*	20	0	0
	16	8	2		17	7	2			13	12	7		16	11	2		16	12	0
	14	8	8		15	9	6			19	1	1		16	10	5	1.	20	1	0
	12	12	6		14	11	5		3	17	7	5		14	13	4		19	6	2
5	18	1	0		13	13	2			13	13	5		14	11	8		16	12	1
	17	6	0		11	11	10			11	11	11		14	11	8		16	9	8
	15	10	0	4*	18	4	2		4	18	6	2	2	18	7	3		14	14	3
	15	8	6		14	12	2		5	19	2	0		15	11	6	2	20	1	1
	12	10	9		12	10	10			18	5	4	4*	16	8	8		19	5	4
6	18	1	1	5	16	8	5			16	10	3	5	18	6	5		17	8	7
	17	6	1		14	10	7			14	13	0		15	12	4		16	11	5
	15	10	1	6	16	9	3			14	12	5	6	19	5	0		13	13	8
	14	11	3		15	11	0			12	11	10		17	9	4	3	15	13	3
	14	9	7		12	11	9		6	19	2	1		16	11	3	4	20	2	0
	13	11	6	7	17	7	3			14	13	1		16	9	7		18	8	4
8*	18	2	0		15	11	1			14	11	7		12	11	11		16	12	2
	16	6	6		13	13	3											14	12	8

TABLE 3.8.6A (continued)

 $s=h^2+k^2+l^2$, \sqrt{s} and mantissa of $\log s$, for $s=8n+p \not\equiv 4^m \cdot 7 \pmod{4^m \cdot 8}$, $m=0, 1, 2, \dots$

$\begin{smallmatrix} p \\ n \end{smallmatrix}$	0	1	2	3	4	5	6
33	264 16.2481 421 604	265 16.2788 423 246	266 16.3095 424 882	267 16.3401 426 511	268 16.3707 428 135	269 16.4012 429 752	270 16.4317 431 364
34	272 16.4924 434 569	273 16.5227 436 163	274 16.5529 437 751	275 16.5831 439 333	276 16.6132 440 909	277 16.6433 442 480	278 16.6733 444 045
35	280 16.7332 447 158	281 16.7631 448 706	282 16.7929 450 249	283 16.8226 451 786		285 16.8819 454 845	286 16.9115 456 366
36	288 16.9706 459 392	289 17.0000 460 898	290 17.0294 462 398	291 17.0587 463 893	292 17.0880 465 383	293 17.1172 466 868	294 17.1464 468 347
37	296 17.2047 471 292	297 17.2337 472 756	298 17.2627 474 216	299 17.2916 475 671	300 17.3205 477 121	301 17.3494 478 566	302 17.3781 480 007
38	304 17.4356 482 874	305 17.4642 484 300	306 17.4929 485 721	307 17.5214 487 138	308 17.5499 488 551	309 17.5784 489 958	310 17.6068 491 362
39	312 17.6635 494 155	313 17.6918 495 544	314 17.7200 496 930	315 17.7482 498 311		317 17.8045 501 059	318 17.8326 502 427
40	320 17.8885 505 150	321 17.9165 506 505	322 17.9444 507 856	323 17.9722 509 203	324 18.0000 510 545	325 18.0278 511 883	326 18.0555 513 218
41	328 18.1108 515 874	329 18.1384 517 196	330 18.1659 518 514	331 18.1934 519 828	332 18.2209 521 138	333 18.2483 522 444	334 18.2757 523 746
42	336 18.3303 526 339	337 18.3576 527 630	338 18.3848 528 917	339 18.4120 530 200	340 18.4391 531 479	341 18.4662 532 754	342 18.4932 534 026
43	344 18.5472 536 558	345 18.5742 537 819	346 18.6011 539 076	347 18.6279 540 329		349 18.6815 542 825	350 18.7083 544 068

TABLE 3.8.6A (continued)

Every s followed by all possible (hkl) triplets

s	h	k	l	s	h	k	l	s	h	k	l	s	h	k	l	s	h	k	l	
405	20	2	1	425	20	5	0	442	21	1	0	459	21	3	3	477*	21	6	0	
	18	9	0		20	4	3		19	9	0		19	7	7		19	10	4	
	17	10	4		19	8	0		17	12	3		17	13	1		18	12	3	
	16	10	7		18	10	1	3	21	1	1		17	11	7		16	14	5	
	15	12	6		17	10	6		19	9	1		15	15	3		16	11	10	
6	19	6	3		16	13	0	5*	15	13	7		13	13	11	8	21	6	1	
	18	9	1		16	12	5		21	2	0						19	9	6	
	17	9	6		15	14	2		20	6	3									
	15	10	9		15	10	10		18	11	0									
8*	20	2	2	6	20	5	1	6	21	2	1	460	18	10	6	480*	20	8	4	
	14	14	4		19	8	1		19	9	2	1	21	4	2	1	21	6	2	
9	20	3	0		19	7	4		19	7	6		20	6	5		20	9	0	
	18	9	2		17	11	4		18	11	1		19	10	0		18	11	6	
	18	7	6		16	13	1		17	11	6		19	8	6		16	15	0	
	16	12	3		16	11	7		15	14	5		18	11	4		16	12	9	
	12	12	11	7	15	11	9		15	11	10		16	14	3	2	21	5	4	
				8	18	10	2		14	13	9		16	13	6		20	9	1	
					14	14	6	9**	21	2	2		14	12	11		19	11	0	
410	20	3	1	9	20	5	2		20	7	0	2	19	10	1		17	12	7	
	19	7	0		19	8	2		18	11	2		17	13	2		16	15	1	
	17	11	0		16	13	2		18	10	5	4*	20	8	0		13	13	12	
	15	13	4		14	13	8		17	12	4		16	12	8	3	19	11	1	
	15	11	8						16	12	7	5	20	8	1		17	13	5	
1	19	7	1	430	18	9	5						20	7	4	4	22	0	0	
	19	5	5		15	14	3						19	10	2		18	12	4	
	17	11	1		15	13	6						14	13	10		14	12	12	
	13	11	11	2*	20	4	4					6	21	5	0	5	22	1	0	
3*	20	3	2		12	12	12	450	21	3	0		21	4	3		20	9	2	
	19	6	4	3	19	6	6		20	7	1		15	15	4		20	7	6	
	18	8	5		18	10	3		20	5	5	7	21	5	1		17	14	0	
	16	11	6		17	12	0		19	8	5		19	9	5		16	15	2	
	13	12	10		15	12	8		16	13	5		17	13	3		15	14	8	
4	19	7	2	4	20	5	3		15	15	0		15	11	11	6	22	1	1	
	18	9	3		19	8	3		15	12	9	8	20	8	2		21	6	3	
	17	11	2		17	12	1	1	21	3	1		18	12	0		19	11	2	
	17	10	5		17	9	8		19	9	3		16	14	4		19	10	5	
	14	13	7		16	13	3		17	9	9	9	18	12	1		18	9	9	
6*	20	4	0		13	12	11		15	15	1		18	9	8		17	14	1	
	16	12	4		19	7	5	2	20	6	4		17	12	6		15	15	6	
7	20	4	1	5	17	11	5		18	8	8		15	12	10	8*	22	2	0	
	17	8	8		20	6	0		16	14	0						18	10	8	
	14	14	5	6	16	12	6		20	7	2						16	14	6	
	14	11	10		20	6	1		17	10	8		470	21	5	2	9	22	2	1
8	20	3	3	7	18	8	7		16	14	1			19	10	3		20	8	5
	16	9	9		17	12	2		21	3	2			18	11	5		19	8	8
	15	12	7		16	10	9		18	11	3			17	10	9		17	14	2
9	19	7	3		15	14	4		18	9	7			15	14	7		17	10	10
	17	11	3		17	10	7		15	15	2	2*	20	6	6		16	13	8	
	17	9	7	8	14	11	11		16	14	2		18	12	2					
	15	13	5		13	13	10		16	10	10	3	21	4	4					
	13	13	9						14	14	8		20	8	3	490	21	7	0	
420	20	4	2	440*	20	6	2	7	21	4	0		18	10	7		20	9	3	
	16	10	8		18	10	4		15	14	6		14	14	9		16	15	3	
1	18	9	4		14	12	10		13	12	12	4	20	7	5		15	12	11	
	15	14	0	1	21	0	0	8	21	4	1		19	8	7	1	21	7	1	
	14	12	9		20	5	4		20	7	3		17	13	4		21	5	5	
2	19	6	5		19	8	4		19	9	4		17	11	8		19	11	3	
	18	7	7		18	9	6		17	13	0		16	13	7		19	9	7	
	15	14	1		16	13	4		17	12	5	5	21	5	3		17	11	9	
4*	18	10	0		16	11	8		16	11	9		15	15	5	2	22	2	2	
	18	8	6		14	14	7		15	13	8		15	13	9		14	14	10	

TABLE 3.8.6A (continued)

 $s=h^2+k^2+l^2$, \sqrt{s} and mantissa of $\log s$, for $s=8n+p \not\equiv 4^m \cdot 7 \pmod{4^m \cdot 8}$, $m=0, 1, 2, \dots$

$\begin{smallmatrix} p \\ n \end{smallmatrix}$	0	1	2	3	4	5	6
44	352 18·7617 546 543	353 18·7883 547 775	354 18·8149 549 003	355 18·8414 550 228	356 18·8680 551 450	357 18·8944 552 668	358 18·9209 553 883
45	360 18·9737 556 303	361 19·0000 557 507	362 19·0263 558 709	363 19·0526 559 907	364 19·0788 561 101	365 19·1050 562 293	366 19·1311 563 481
46		369 19·2094 567 026	370 19·2354 568 202	371 19·2614 569 374	372 19·2873 570 543	373 19·3132 571 709	374 19·3391 572 872
47	376 19·3907 575 188	377 19·4165 576 341	378 19·4422 577 492	379 19·4679 578 639		381 19·5192 580 925	382 19·5448 582 063
48	384 19·5959 584 331	385 19·6214 585 461	386 19·6469 586 587	387 19·6723 587 711	388 19·6977 588 832	389 19·7231 589 950	390 19·7484 591 065
49	392 19·7990 593 286	393 19·8242 594 393	394 19·8494 595 496	395 19·8746 596 597	396 19·8997 597 695	397 19·9249 598 791	398 19·9499 599 883
50	400 20·0000 602 060	401 20·0250 603 144	402 20·0499 604 226	403 20·0749 605 305	404 20·0998 606 381	405 20·1246 607 455	406 20·1494 608 526
51	408 20·1990 610 660	409 20·2237 611 723	410 20·2485 612 784	411 20·2731 613 842		413 20·3224 615 950	414 20·3470 617 000
52	416 20·3961 619 093	417 20·4206 620 136	418 20·4450 621 176	419 20·4695 622 214	420 20·4939 623 249	421 20·5183 624 282	422 20·5426 625 312
53	424 20·5913 627 366	425 20·6155 628 389	426 20·6398 629 410	427 20·6640 630 428	428 20·6882 631 444	429 20·7123 632 457	430 20·7364 633 468
54	432 20·7846 635 484	433 20·8087 636 488	434 20·8327 637 490	435 20·8567 638 489	436 20·8806 639 486	437 20·9045 640 481	438 20·9284 641 474

TABLE 3.8.6A (continued)

Every s followed by all possible (hkl) triplets																				
s	h	k	l	s	h	k	l	s	h	k	l	s	h	k	l	s	h	k	l	
493	22	3	0	510	22	5	1	528*	20	8	8	545	23	4	0	561	23	4	4	
	21	6	4		19	10	7		16	16	4		22	6	5		19	14	2	
	18	13	0		17	14	5	9	23	0	0		21	10	2		19	10	10	
	18	12	5		17	11	10		22	6	3		20	12	1		17	16	4	
4	22	3	1	2*	16	16	0		18	14	3		20	9	8		16	16	7	
	21	7	2	3	22	5	2		18	13	6		18	14	5		14	14	13	
	18	13	1		21	6	6						18	11	10	2	21	11	0	
	18	11	7		20	8	7						17	16	0		20	9	9	
	17	14	3		16	16	1	530	23	1	0		16	15	8		16	15	9	
	17	13	6		15	12	12		21	8	5		6	23	4	1	3	23	5	3
	15	13	10		14	14	11		20	11	3			20	11	5		21	11	1
7**	22	3	2	4	21	8	3		20	9	7			19	13	4		19	11	9
	20	9	4		19	12	3		19	13	0			19	11	8		17	15	7
	19	10	6		17	15	0		19	12	5			17	16	1		15	13	13
	18	13	2		17	12	9		17	15	4			16	13	11	4	22	8	4
	17	12	8		15	15	8		16	15	7	7	23	3	3		20	10	8	
	16	15	4	5	21	7	5	1	23	1	1		21	9	5	5	23	6	0	
8	20	7	7		17	15	1		21	9	3	8	22	8	0		22	9	0	
	19	11	4		15	13	11		19	13	1		20	12	2		18	15	4	
	16	11	11	6	22	4	4		19	11	7		16	16	6		15	14	12	
9	21	7	3		20	10	4		17	11	11	9	23	4	2	6	23	6	1	
	15	15	7		16	16	2		15	15	9		22	8	1		22	9	1	
					16	14	8		2	18	12	8	22	7	4		21	11	2	
				7	20	9	6	3	23	2	0		20	10	7		21	10	5	
					18	12	7		22	7	0		18	15	0		19	14	3	
					16	15	6		17	12	10		18	12	9		19	13	6	
500	22	4	0	8	22	5	3	4	23	2	1		17	16	2		18	11	11	
	20	10	0		19	11	6		22	7	1		17	14	8		17	14	9	
	20	8	6		18	13	5		22	5	5					8*	18	12	10	
	16	12	10		17	15	2		19	13	2					9	23	6	2	
1	22	4	1						17	14	7		550	21	10	3	22	9	2	
	20	10	1						14	13	13			18	15	1	22	7	6	
	17	14	4					6*	22	6	4			17	15	6	21	8	8	
	16	14	7						20	10	6			15	15	10	20	13	0	
2	22	3	3	520*	22	6	0		18	14	4		2*	22	8	2	20	12	5	
	21	6	5		18	14	0		14	14	12		3	20	12	3	19	12	8	
	18	13	3	1	22	6	1		23	2	2			18	15	2	18	14	7	
	15	14	9		21	8	4	7	22	7	2		4	23	5	0	16	13	12	
4*	22	4	2		20	11	0		20	11	4			23	4	3				
	20	10	2		19	12	4		16	16	5			21	8	7				
	18	12	6		18	14	1	8	23	3	0			19	12	7				
5	21	8	0		17	14	6		21	9	4			17	16	3				
	19	12	0		16	16	3		15	13	12			17	12	11	570	23	5	4
	18	10	9		15	14	10		23	3	1	5	23	5	1		20	13	1	
6	21	8	1		21	9	0	9	21	7	7		19	13	5		20	11	7	
	20	9	5	2	20	11	1		19	13	3		6	22	6	6	1	17	16	5
	19	12	1		17	13	8		17	15	5			18	14	6		21	11	3
	19	9	8	3	21	9	1		17	13	9	7	22	8	3		21	9	7	
	16	15	5		19	9	9						21	10	4	3*	22	8	5	
	16	13	9		17	15	3						20	11	6		20	13	2	
7	19	11	5	4	22	6	2	541*	21	10	0		19	14	0		19	14	4	
	17	13	7		18	14	2		21	8	6			18	13	8		16	14	11
	13	13	13		18	10	10		19	12	6		8	23	5	2	4	23	6	3
9*	22	5	0	5	22	5	4	2	23	3	2			22	7	5		22	9	3
	22	4	3		20	11	2		22	7	3			21	9	6		18	15	5
	21	8	2		20	10	5		21	10	1			19	14	1		18	13	9
	20	10	3		19	10	8		19	10	9			18	15	3	6*	24	0	0
	19	12	2		16	13	10		18	13	7			17	13	10		16	16	8
	18	13	4	6	21	9	2		15	14	11					7	24	1	0	
	18	11	8		21	7	6	4*	20	12	0						21	10	6	
	14	13	12		18	11	9		16	12	12		560*	20	12	4		17	12	12

TABLE 3.8.6A (continued)

 $s = h^2 + k^2 + l^2$, \sqrt{s} and mantissa of $\log s$, for $s = 8n + p \not\equiv 4^m \cdot 7 \pmod{4^m \cdot 8}$, $m = 0, 1, 2, \dots$

$p \backslash n$	0	1	2	3	4	5	6
55	440 20·9762 643 453	441 21·0000 644 439	442 21·0238 645 422	443 21·0476 646 404		445 21·0950 648 360	446 21·1187 649 335
56		449 21·1896 652 246	450 21·2132 653 213	451 21·2368 654 177	452 21·2603 655 138	453 21·2838 656 098	454 21·3073 657 056
57	456 21·3542 658 965	457 21·3776 659 916	458 21·4009 660 865	459 21·4243 661 813	460 21·4476 662 758	461 21·4709 663 701	462 21·4942 664 642
58	464 21·5407 666 518	465 21·5639 667 453	466 21·5870 668 386	467 21·6102 669 317	468 21·6333 670 246	469 21·6564 671 173	470 21·6795 672 098
59	472 21·7256 673 942	473 21·7486 674 861	474 21·7715 675 778	475 21·7945 676 694		477 21·8403 678 518	478 21·8632 679 428
60	480 21·9089 681 241	481 21·9317 682 145	482 21·9545 683 047	483 21·9773 683 947	484 22·0000 684 845	485 22·0227 685 742	486 22·0454 686 636
61	488 22·0907 688 420	489 22·1133 689 309	490 22·1359 690 196	491 22·1585 691 081	492 22·1811 691 965	493 22·2036 692 847	494 22·2261 693 727
62		497 22·2935 696 356	498 22·3159 697 229	499 22·3383 698 100	500 22·3607 698 970	501 22·3830 699 838	502 22·4054 700 704
63	504 22·4499 702 431	505 22·4722 703 291	506 22·4944 704 151	507 22·5167 705 008		509 22·5610 706 718	510 22·5832 707 570
64	512 22·6274 709 270	513 22·6495 710 117	514 22·6716 710 963	515 22·6936 711 807	516 22·7156 712 650	517 22·7376 713 491	518 22·7596 714 330
65	520 22·8035 716 003	521 22·8254 716 838	522 22·8473 717 671	523 22·8692 718 502	524 22·8910 719 331	525 22·9129 720 159	526 22·9347 720 986

TABLE 3.8.6A (continued)

Every s followed by all possible (hkl) triplets

s	h	k	l	s	h	k	l	s	h	k	l	s	h	k	l	s	h	k	l
578	24	1	1	593	24	4	1	609	23	8	4	626	25	1	0	641	25	4	0
	23	7	0		23	8	0		22	11	2		24	7	1		24	8	1
	21	11	4		22	10	3		22	10	5		24	5	5		24	7	4
	20	13	3		20	12	7		17	16	8		23	9	4		22	11	6
	17	17	0		19	14	6						21	13	4		21	14	2
	17	15	8		18	13	10	610	24	5	3		21	11	8		21	10	10
9	23	7	1		16	16	9		23	9	0		20	15	1		20	15	4
	23	5	5	4	24	3	3		21	13	0		19	16	3		18	14	11
	19	13	7		23	8	1		21	12	5		19	12	11	2	25	4	1
	17	17	1		23	7	4	1	23	9	1		17	16	9		23	8	7
	17	13	11		21	12	3		21	13	1	7	25	1	1		20	11	11
					20	13	5		21	11	7		23	7	7		19	16	5
					19	13	8		19	15	5		17	17	7		17	17	8
580	24	2	0		17	17	4		19	13	9		17	13	13	3	25	3	3
	20	12	6		17	16	7	2	24	6	0	8	24	6	4		21	11	9
	18	16	0		16	13	13		22	8	8		22	12	0	4	24	8	2
1	24	2	1		15	15	12		20	14	4	9	25	2	0		22	12	4
	23	6	4	5	19	15	3		18	12	12		24	7	2		20	12	10
	22	9	4		17	15	9		16	16	10		23	10	0		18	16	8
	20	10	9	6	24	4	2	3	24	6	1		23	8	6	5	25	4	2
	18	16	1		20	14	0		18	17	0		22	12	1		23	10	4
	17	16	6		18	16	4		18	15	8		22	9	8		20	14	7
	16	15	10		16	14	12	4	23	9	2		20	15	2		17	16	10
2	23	7	2		23	8	2		23	7	6		18	17	4	6	23	9	6
	22	7	7	7	22	8	7		22	11	3		18	16	7		22	9	9
	19	14	5		20	14	1		22	9	7		17	14	12		21	14	3
	19	11	10		21	11	6	8	21	13	2						21	13	6
	17	17	2		18	15	7		18	17	1						15	15	14
4*	24	2	2						18	13	11	630	25	2	1	8*	24	6	6
	22	10	0						17	17	6		23	10	1		22	10	8
	22	8	6						17	15	10		22	11	5		18	18	0
	18	16	2	600*	22	10	4	6*	24	6	2		19	13	10		16	14	14
	18	14	8		20	14	2		18	16	6		18	15	9	9	24	8	3
5	24	3	0		20	10	10	7	24	5	4	2*	22	12	2		21	12	8
	22	10	1	1	24	5	0		19	16	0		20	14	6		19	12	12
	21	12	0		24	4	3		18	17	2	3	25	2	2		18	18	1
	20	13	4		23	6	6		15	14	14		23	10	2		18	17	6
	20	11	8		22	9	6	8	23	8	5		22	10	7		18	15	10
	18	15	6		21	12	4		20	13	7		20	13	8				
	17	14	10		18	14	9		19	16	1		19	16	4				
6	24	3	1	2	24	5	1	9	23	9	3	4	16	16	11	650	25	5	0
	21	12	1		23	8	3		21	13	3		25	3	0		25	4	3
	21	9	8		20	11	9		15	15	13		24	7	3		24	7	5
	19	15	0		19	15	4						21	12	7		23	11	0
	19	12	9		17	13	12	620	22	10	6		20	15	3		20	15	5
7	23	7	3		16	15	11	1	24	6	3	5	25	3	1		20	13	9
	21	11	5	3	23	7	5		22	11	4		23	9	5		19	17	0
	19	15	1		21	9	9		21	12	6		21	13	5		19	15	8
	17	17	3		19	11	11		20	14	5		19	15	7		16	15	13
8	22	10	2		17	17	5		20	11	10	7*	17	15	11	1	25	5	1
	14	14	14	5*	24	5	2		19	16	2		24	6	5		23	11	1
9	24	3	2		22	11	0		19	14	8		22	12	3		19	17	1
	21	12	2		21	10	8		16	14	13		21	14	0		19	13	11
	18	16	3		20	14	3	2	21	10	9	8	18	13	12	2	18	18	2
	18	12	11		20	13	6		19	15	6		25	3	2	3	22	13	0
					19	12	10		18	17	3		23	10	3		22	12	5
590	23	6	5	6	22	11	1	5**	25	0	0		21	14	1		21	14	4
	22	9	5		19	14	7		24	7	0		19	14	9		19	16	6
	21	10	7		17	14	11		20	15	0		18	17	5				
	19	15	2	8*	24	4	4		20	12	9								
2*	15	14	13		20	12	8		16	15	12	640*	24	8	0				
	24	4	0																

TABLE 3.8.6A (continued)

 $s = h^2 + k^2 + l^2$, \sqrt{s} and mantissa of $\log s$, for $s = 8n + p \neq 4^m \cdot 7 \pmod{4^m \cdot 8}$, $m = 0, 1, 2, \dots$

$\begin{array}{c} p \\ n \end{array}$	0	1	2	3	4	5	6
66	528 22.9783 722 634	529 23.0000 723 456	530 23.0217 724 276	531 23.0434 725 095	532 23.0651 725 912	533 23.0868 726 727	534 23.1084 727 541
67	536 23.1517 729 165	537 23.1733 729 974	538 23.1948 730 782	539 23.2164 731 589		541 23.2594 733 197	542 23.2809 733 999
68	544 23.3238 735 599	545 23.3452 736 397	546 23.3666 737 193	547 23.3880 737 987	548 23.4094 738 781	549 23.4307 739 572	550 23.4521 740 363
69	552 23.4947 741 939	553 23.5160 742 725	554 23.5372 743 510	555 23.5584 744 293	556 23.5797 745 075	557 23.6008 745 855	558 23.6220 746 634
70	560 23.6643 748 188	561 23.6854 748 963	562 23.7065 749 736	563 23.7276 750 508	564 23.7487 751 279	565 23.7697 752 048	566 23.7908 752 816
71	568 23.8328 754 348	569 23.8537 755 112	570 23.8747 755 875	571 23.8956 756 636		573 23.9374 758 155	574 23.9583 758 912
72	576 24.0000 760 422	577 24.0208 761 176	578 24.0416 761 928	579 24.0624 762 679	580 24.0832 763 428	581 24.1039 764 176	582 24.1247 764 923
73	584 24.1661 766 413	585 24.1868 767 156	586 24.2074 767 898	587 24.2281 768 638	588 24.2487 769 377	589 24.2693 770 115	590 24.2899 770 852
74	592 24.3311 772 322	593 24.3516 773 055	594 24.3721 773 786	595 24.3926 774 517	596 24.4131 775 246	597 24.4336 775 974	598 24.4540 776 701
75	600 24.4949 778 151	601 24.5153 778 874	602 24.5357 779 596	603 24.5561 780 317		605 24.5967 781 755	606 24.6171 782 473
76	608 24.6577 783 904	609 24.6779 784 617	610 24.6982 785 330	611 24.7184 786 041	612 24.7386 786 751	613 24.7588 787 460	614 24.7790 788 168

TABLE 3.8.6A (continued)

Every s followed by all possible (hkl) triplets

s	h	k	l	s	h	k	l	s	h	k	l	s	h	k	l	s	h	k	l	
654	25	5	2	670	25	6	3	685	26	3	0	699	25	7	5	714	25	8	5	
	23	11	2		21	15	2		24	10	3		23	13	1		23	13	4	
	23	10	5		18	15	11		21	12	10		23	11	7		23	11	8	
	22	13	1	2*	20	16	4		19	18	0		19	17	7		20	17	5	
	22	11	7	3	24	9	4	6	26	3	1		19	13	13		19	17	8	
	19	17	2		23	12	0		25	6	5		17	17	11		17	16	13	
	17	14	13		21	14	6		23	11	6					5	25	9	3	
6*	24	8	4		18	18	5		22	11	9						21	15	7	
	20	16	0	4	25	7	0		21	14	7	701*	26	5	0	6	26	6	2	
	16	16	12		24	7	7		19	18	1		26	4	3		22	14	6	
7	25	4	4		23	12	1		19	17	6		24	11	2		18	14	14	
	24	9	0		23	9	8		19	15	10		24	10	5	7	26	5	4	
	23	8	8		21	13	8	8*	20	12	12		21	16	2		22	13	8	
	22	13	2		20	15	7	9	26	3	2		21	14	8		20	14	11	
	20	16	1		19	13	12		25	8	0		19	18	4		19	16	10	
	19	14	10	5	25	7	1		24	8	7		19	14	12	8	22	15	3	
	18	18	3		25	5	5		23	12	4		18	16	11		21	14	9	
8	24	9	1		23	11	5		22	14	3	2	26	5	1		18	15	13	
	17	15	12		21	15	3		22	13	6		23	13	2					
9	25	5	3		19	17	5		20	17	0		22	13	7					
	23	11	3		15	15	15		20	15	8	4*	21	15	6					
	23	9	7	6	26	0	0		19	18	2	5	24	8	8	720*	24	12	0	
	21	13	7		24	10	0		18	14	13		26	5	2		20	16	8	
	19	17	3		24	8	6		17	16	12		25	8	4	1	26	6	3	
	17	17	9	7	26	1	0						22	14	5		24	12	1	
					25	6	4						22	11	10		24	9	8	
					24	10	1						20	17	4		19	18	6	
660	20	16	2		23	12	2	690	25	8	1		20	16	7	2	25	9	4	
	20	14	8		22	12	7		25	7	4		25	9	0		24	11	5	
1	25	6	0		20	14	9		20	17	1		24	11	3		23	12	7	
	24	9	2		18	17	8		20	13	11		24	9	7		21	16	5	
	24	7	6		16	15	14		1	23	9	9	21	16	3		19	19	0	
	20	15	6	8	26	1	1			21	15	5	21	12	11		17	17	12	
	18	16	9		25	7	2			21	13	9	20	15	9	3	25	7	7	
2	25	6	1		23	10	7		2	26	4	0	7	16	15	15	23	13	5	
	22	13	3		22	13	5			24	10	4		25	9	1	19	19	1	
	21	14	5		19	14	11			22	12	8		23	13	3	4	24	12	2
	21	11	10		17	17	10			20	16	6	8	19	15	11		20	18	0
	18	17	7							26	4	1		26	4	4		18	16	12
	18	13	13							25	8	2	9	16	16	14	5	26	7	0
4*	22	12	6							24	9	6		23	12	6		25	10	0
	18	18	4							23	10	8		22	15	0		25	8	6
	18	14	12	680*	26	2	0			20	17	2		22	12	9		24	10	7
5	25	6	2		24	10	2			18	15	12						23	14	0
	24	8	5		22	14	0		4	26	3	3		710	26	5	3	22	15	4
	23	10	6		18	16	10			19	18	3			25	9	2	20	18	1
	22	10	9	1	26	2	1			18	17	9			25	7	6	20	17	6
	20	16	3		22	14	1			26	4	2			23	10	9	20	15	10
	20	12	11		20	16	5		6*	22	14	4			22	15	1	26	7	1
6	25	5	4		19	16	8			20	14	10			21	13	10	26	5	5
	24	9	3		17	14	14		7	25	6	6			19	18	5	25	10	1
	23	11	4		16	16	13			24	11	0		2*	17	15	14	23	14	1
	21	15	0	2	24	9	5			21	16	0			26	6	0	22	11	11
	21	12	9		23	12	3			18	18	7			24	10	6	19	19	2
	19	17	4		21	15	4		8	25	8	3		3	18	18	8	19	14	13
	19	16	7	3	25	7	3			24	11	1			26	6	1	26	6	4
	17	16	11		21	11	11			23	13	0			24	11	4	22	12	10
7	21	15	1		17	15	13			23	12	5			22	15	2	20	18	2
	19	15	9	4	26	2	2			21	16	1			21	16	4			
9*	22	13	4		22	14	2			20	17	3			20	13	12			
	22	11	8		22	10	10			19	16	9			18	17	10			
	20	13	10		18	18	6													

TABLE 3.8.6A (continued)

 $s = h^2 + k^2 + l^2$, \sqrt{s} and mantissa of $\log s$, for $s = 8n + p \neq 4^m \cdot 7 \pmod{4^m \cdot 8}$, $m = 0, 1, 2, \dots$

$\begin{array}{c} p \\ n \end{array}$	0	1	2	3	4	5	6
77	616 24.8193 789 581	617 24.8395 790 285	618 24.8596 790 988	619 24.8797 791 691	620 24.8998 792 392	621 24.9199 793 092	622 24.9399 793 790
78		625 25.0000 795 880	626 25.0200 796 574	627 25.0400 797 268	628 25.0599 797 960	629 25.0799 798 651	630 25.0998 799 341
79	632 25.1396 800 717	633 25.1595 801 404	634 25.1794 802 089	635 25.1992 802 774		637 25.2389 804 139	638 25.2587 804 821
80	640 25.2982 806 180	641 25.3180 806 858	642 25.3377 807 535	643 25.3574 808 211	644 25.3772 808 886	645 25.3969 809 560	646 25.4165 810 233
81	648 25.4558 811 575	649 25.4755 812 245	650 25.4951 812 913	651 25.5147 813 581	652 25.5343 814 248	653 25.5539 814 913	654 25.5734 815 578
82	656 25.6125 816 904	657 25.6320 817 565	658 25.6515 818 226	659 25.6710 818 885	660 25.6905 819 544	661 25.7099 820 201	662 25.7294 820 858
83	664 25.7682 822 168	665 25.7876 822 822	666 25.8070 823 474	667 25.8263 824 126		669 25.8650 825 426	670 25.8844 826 075
84	672 25.9230 827 369	673 25.9422 828 015	674 25.9615 828 660	675 25.9808 829 304	676 26.0000 829 947	677 26.0192 830 589	678 26.0384 831 230
85	680 26.0768 832 509	681 26.0960 833 147	682 26.1151 833 784	683 26.1343 834 421	684 26.1534 835 056	685 26.1725 835 691	686 26.1916 836 324
86	688 26.2298 837 588	689 26.2488 838 219	690 26.2679 838 849	691 26.2869 839 478	692 26.3059 840 106	693 26.3249 840 733	694 26.3439 841 359
87	696 26.3818 842 609	697 26.4008 843 233	698 26.4197 843 855	699 26.4386 844 477		701 26.4764 845 718	702 26.4953 846 337

TABLE 3.8.6A (continued)

Every s followed by all possible (hkl) triplets

s	h	k	l	s	h	k	l	s	h	k	l	s	h	k	l	s	h	k	l			
729	27	0	0	741	26	8	1	755	27	5	1	770	27	5	4	782	27	7	2			
	26	7	2		26	7	4		25	11	3		25	12	1		26	9	5			
	25	10	2		25	10	4		25	9	7		25	9	8		25	11	6			
	24	12	3		23	14	4		23	15	1		24	13	5		22	17	3			
	23	14	2		22	16	1		21	17	5		23	15	4		19	15	14			
	23	10	10		17	16	14		19	15	13		20	19	3		18	17	13			
	22	14	7	2	27	3	2	6	26	8	4		20	17	9	4*	28	0	0			
	21	12	12		25	9	6		24	12	6		17	16	15		24	12	8			
	18	18	9	4*	26	8	2		22	16	4	1	25	11	5	5	28	1	0			
					22	16	2		20	16	10		23	11	11		26	10	3			
					22	14	8		7	26	9	0	19	19	7		25	12	4			
				5	27	4	0		24	10	9		19	17	11		23	16	0			
					24	13	0		18	17	12	2	24	14	0		19	18	10			
730	27	1	0		24	12	5	8	27	5	2		22	12	12	6	28	1	1			
	21	17	0		22	15	6		26	9	1	3	26	9	4		23	16	1			
	21	15	8		18	15	14		23	15	2		25	12	2		20	19	5			
	19	15	12		27	4	1		22	15	7		24	14	1		19	19	8			
1	27	1	1	6	25	11	0		21	14	11		23	12	10		19	16	13			
	25	9	5		24	13	1		19	19	6		22	17	0	7	27	7	3			
	23	11	9		24	11	7						22	15	8		25	9	9			
	21	17	1		21	17	4						20	18	7		21	15	11			
	21	13	11		21	16	7		760*	20	18	6	4	27	6	3	8	28	2	0		
	19	19	3		20	15	11		1	27	4	4		26	7	7		24	14	4		
	19	17	9		27	3	3			26	9	2		25	10	7		20	18	8		
3*	27	2	0	7	25	11	1			26	7	6		23	14	7	9	28	2	1		
	24	11	6		23	13	7			25	10	6		22	17	1		26	8	7		
	21	16	6		21	15	9			24	13	4		22	13	11		25	10	8		
	20	18	3		19	19	5			24	11	8		21	18	3		23	16	2		
4	27	2	1		17	17	13			23	14	6		18	15	15		23	14	8		
	26	7	3		26	6	6			22	14	9	6*	17	17	14		22	17	4		
	25	10	3	8	18	18	10			21	16	8		26	10	0		22	16	7		
	23	14	3		27	4	2			20	19	0		26	8	6		20	17	10		
	23	13	6	9	26	8	3			19	16	12		24	14	2						
	22	15	5		24	13	2			25	11	4		24	10	10						
	22	13	9		22	16	3		2	23	13	8		22	16	6						
	21	17	2		22	12	11			20	19	1		18	16	14		790	27	6	5	
	19	18	7		20	18	5			27	5	3		26	10	1			23	15	6	
	18	17	11		19	18	8		3	23	15	3		22	17	2			22	15	9	
6*	24	12	4		18	16	13			27	6	0		20	19	4			21	18	5	
7	27	2	2						5*	26	8	5		20	16	11	2*	28	2	2		
	26	6	5							22	16	5		27	7	0			26	10	4	
	23	12	8							21	18	0		25	12	3			20	14	14	
	21	14	10							20	19	2		24	11	9			18	18	12	
	20	16	9							20	14	13		21	16	9	3		28	3	0	
8	27	3	0						6	27	6	1		27	7	1			27	8	0	
	25	8	7							26	9	3		27	5	5			26	9	6	
	24	9	9							21	18	1		23	15	5	4		28	3	1	
	20	17	7							21	17	6		23	13	9			27	8	1	
	20	13	13		3**	25	8	8		21	15	10		21	17	7			27	7	4	
	19	19	4			22	13	10		19	18	9		21	13	13			25	13	0	
	19	16	11			20	17	8		16	16	16							25	12	5	
9	27	3	1			19	14	14	8*										24	13	7	
	21	17	3		4	27	5	0	9	27	6	2							23	16	3	
	17	15	15			27	4	3		25	12	0		780	26	10	2		23	12	11	
						24	13	3		24	12	7			22	14	10			21	17	8
						23	15	0		21	18	2		1	27	6	4			20	15	13
						23	12	9		20	15	12			24	14	3			19	17	12
						21	13	12		18	18	11			24	13	6			25	13	1
740	26	8	0												21	18	4		5	25	11	7
	24	10	8												21	14	12					
	22	16	0																			
	20	18	4																			
	20	14	12																			

TABLE 3.8.6A (continued)

 $s=h^2+k^2+l^2$, \sqrt{s} and mantissa of $\log s$, for $s=8n+p \neq 4^m \cdot 7 \pmod{4^m \cdot 8}$, $m=0, 1, 2, \dots$

$n \backslash p$	0	1	2	3	4	5	6
88	704 26.5330 847 573	705 26.5518 848 189	706 26.5707 848 805	707 26.5895 849 419	708 26.6083 850 033	709 26.6271 850 646	710 26.6458 851 258
89	712 26.6833 852 480	713 26.7021 853 090	714 26.7208 853 698	715 26.7395 854 306	716 26.7582 854 913	717 26.7769 855 519	718 26.7955 856 124
90	720 26.8328 857 332	721 26.8514 857 935	722 26.8701 858 537	723 26.8887 859 138	724 26.9072 859 739	725 26.9258 860 338	726 26.9444 860 937
91	728 26.9815 862 131	729 27.0000 862 728	730 27.0185 863 323	731 27.0370 863 917		733 27.0740 865 104	734 27.0924 865 696
92	736 27.1293 866 878	737 27.1477 867 467	738 27.1662 868 056	739 27.1846 868 644	740 27.2029 869 232	741 27.2213 869 818	742 27.2397 870 404
93	744 27.2764 871 573	745 27.2947 872 156	746 27.3130 872 739	747 27.3313 873 321	748 27.3496 873 902	749 27.3679 874 482	750 27.3861 875 061
94		753 27.4408 876 795	754 27.4591 877 371	755 27.4773 877 947	756 27.4955 878 522	757 27.5136 879 096	758 27.5318 879 669
95	760 27.5681 880 814	761 27.5862 881 385	762 27.6043 881 955	763 27.6225 882 525		765 27.6586 883 661	766 27.6767 884 229
96	768 27.7128 885 361	769 27.7308 885 926	770 27.7489 886 491	771 27.7669 887 054	772 27.7849 887 617	773 27.8029 888 179	774 27.8209 888 741
97	776 27.8568 889 862	777 27.8747 890 421	778 27.8927 890 980	779 27.9106 891 537	780 27.9285 892 095	781 27.9464 892 651	782 27.9643 893 207
98	784 28.0000 894 316	785 28.0179 894 870	786 28.0357 895 423	787 28.0535 895 975	788 28.0713 896 526	789 28.0891 897 077	790 28.1069 897 627

TABLE 3.8.6A (continued)

Every s followed by all possible (hkl) triplets

s	h	k	l	s	h	k	l	s	h	k	l	s	h	k	l	s	h	k	l
797*	28	3	2	809	28	5	0	822	26	11	5	837	28	7	2	850	29	3	0
	27	8	2		28	4	3		25	14	1		25	14	4		27	11	0
	26	11	0		27	8	4		23	17	2		24	15	6		25	15	0
	24	14	5		24	13	8		22	17	7		22	17	8		25	12	9
	24	11	10		22	18	1		22	13	13	8	27	10	3		24	15	7
	22	13	12		22	17	6		19	19	10		26	9	9		21	20	3
	21	16	10		22	15	10	4*	28	6	2		21	19	6		20	15	15
	20	19	6		20	20	3		26	12	2		18	17	15	1	29	3	1
8	26	11	1		18	17	14		22	18	4						27	11	1
	25	13	2						22	14	12						25	15	1
	23	13	10	810	28	5	1		20	18	10						21	19	7
	22	17	5		27	9	0	5	28	5	4	840*	26	10	8		21	17	11
					25	13	4		26	10	7		22	16	10	2	28	8	2
					25	11	8		25	14	2	1	29	0	0		20	16	14
800*	28	4	0		24	15	3		25	10	10		24	16	3	3	24	14	9
	20	20	0		23	16	5		23	14	10		24	12	11		23	18	0
	20	16	12		21	15	12		20	20	5		21	20	0		22	15	12
1	28	4	1		20	19	7		20	19	8		21	16	12	4	29	3	2
	27	6	6		20	17	11		20	16	13		28	1	0		27	11	2
	26	11	2	1	27	9	1	6	27	9	4		27	7	3		27	10	5
	26	10	5		21	19	3		24	15	5		27	8	7		26	13	3
	24	15	0		21	17	9		24	13	9		23	13	12		25	15	2
	24	12	9		19	15	15	7	27	7	7		21	20	1		23	18	1
	23	16	4	2	26	10	6		25	11	9		20	19	9		23	17	6
	22	14	11		22	18	2		23	17	3		19	16	15		23	15	10
	21	18	6	3	28	5	2		21	19	5	3	29	1	1		22	19	3
	20	20	1		26	11	4		19	16	14		25	13	7		22	17	9
	17	16	16		19	16	14		27	10	0		19	19	11	6*	19	18	13
2	28	3	3	4	27	9	2		27	8	6		18	18	14		28	6	6
	27	8	3		27	7	6		26	12	3		22	18	6	7	26	12	6
	24	15	1		21	18	7		21	18	8		18	18	14		29	4	0
	21	19	0	6*	28	4	4		19	18	12		29	2	0		28	8	3
3	27	7	5		20	20	4					5	28	6	5		27	8	8
	25	13	3	7	24	15	4	830	27	10	1		27	10	4		26	10	9
	23	15	7		23	12	12		25	14	3		26	13	0		25	14	6
	21	19	1		22	18	3		25	13	6		26	12	5		24	16	5
	19	19	9		18	18	13		22	15	11		24	13	10		23	18	2
	17	17	15	8	28	5	3		21	17	10		22	19	0		22	18	7
4	28	4	2		27	8	5	2*	24	16	0		21	20	2	8	21	20	4
	26	8	8		25	12	7	3	28	7	0		20	18	11		29	4	1
	22	16	8		24	11	11		27	10	2		29	2	1		28	7	5
	20	20	2		23	17	0		26	11	6	6	27	9	6		25	13	8
5	25	12	6		23	15	8		25	12	8		26	13	1		20	17	13
	24	15	2		21	19	4		24	16	1		26	11	7	9	29	3	3
	20	18	9		21	16	11		22	18	5		25	14	5		27	11	3
	18	16	15	9	27	9	3		21	14	14		25	11	10		27	9	7
6	26	11	3		25	13	5		20	17	12		23	14	11		25	15	3
	26	9	7		23	17	1	4	28	7	1		22	19	1				
	25	10	9		23	13	11		28	5	5		21	18	9				
	23	14	9		19	17	13		23	17	4		19	17	14				
	21	19	2						23	16	7	8*	28	8	0	861*	29	4	2
	21	14	13	820	28	6	0		17	17	16		24	16	4		26	13	4
	19	18	11		26	12	0		27	9	5	9	29	2	2		26	11	8
8*	24	14	6		24	12	10		23	15	9		28	8	1		22	19	4
	22	18	0	1	28	6	1		21	15	13		28	7	4		22	16	11
					26	12	1	6	28	6	4		26	13	2		20	19	10
					26	9	8		26	12	4		23	16	8	2	23	18	3
					25	14	0		24	16	2		22	19	2		21	15	14
					24	14	7		24	14	8		22	14	13	4*	28	8	4
					23	16	6		20	20	6		20	20	7		24	12	12
					22	16	9		18	16	16						20	20	8
					20	15	14												

TABLE 3.8.6A (continued)

 $s = h^2 + k^2 + l^2$, \sqrt{s} and mantissa of $\log s$, for $s = 8n + p \neq 4^m \cdot 7 \pmod{4^m \cdot 8}$, $m = 0, 1, 2, \dots$

$\begin{matrix} p \\ n \end{matrix}$	0	1	2	3	4	5	6
99	792 28.1425 898 725	793 28.1603 899 273	794 28.1780 899 821	795 28.1957 900 367		797 28.2312 901 458	798 28.2489 902 003
100	800 28.2843 903 090	801 28.3019 903 633	802 28.3196 904 174	803 28.3373 904 716	804 28.3549 905 256	805 28.3725 905 796	806 28.3901 906 335
101	808 28.4253 907 411	809 28.4429 907 949	810 28.4605 908 485	811 28.4781 909 021	812 28.4956 909 556	813 28.5132 910 091	814 28.5307 910 624
102	816 28.5657 911 690	817 28.5832 912 222	818 28.6007 912 753	819 28.6182 913 284	820 28.6356 913 814	821 28.6531 914 343	822 28.6705 914 872
103	824 28.7054 915 927	825 28.7228 916 454	826 28.7402 916 980	827 28.7576 917 506		829 28.7924 918 555	830 28.8097 919 078
104	832 28.8444 920 123	833 28.8617 920 645	834 28.8791 921 166	835 28.8964 921 686	836 28.9137 922 206	837 28.9310 922 725	838 28.9482 923 244
105	840 28.9828 924 279	841 29.0000 924 796	842 29.0172 925 312	843 29.0345 925 828	844 29.0517 926 342	845 29.0689 926 857	846 29.0861 927 370
106	848 29.1204 928 396	849 29.1376 928 908	850 29.1548 929 419	851 29.1719 929 930	852 29.1890 930 440	853 29.2062 930 949	854 29.2233 931 458
107	856 29.2575 932 474	857 29.2746 932 981	858 29.2916 933 487	859 29.3087 933 993		861 29.3428 935 003	862 29.3598 935 507
108	864 29.3939 936 514	865 29.4109 937 016	866 29.4279 937 518	867 29.4449 938 019	868 29.4618 938 520	869 29.4788 939 020	870 29.4958 939 519
109	872 29.5296 940 516	873 29.5466 941 014	874 29.5635 941 511	875 29.5804 942 008	876 29.5973 942 504	877 29.6142 943 000	878 29.6311 943 495

TABLE 3.8.6A (continued)

Every s followed by all possible (hkl) triplets

Every s followed by all possible (hkl) triplets																								
s	h	k	l	s	h	k	l	s	h	k	l	s	h	k	l	s	h	k	l					
865	28	9	0	877	29	6	0	891	29	7	1	905	30	2	1	917	30	4	1					
	27	10	6			27	12		2		29		5	5			29	8	0		26	15	4	
	24	17	0			21	20		6		27		9	9			28	11	0		25	16	6	
	24	15	8		8	29	6		1		23		19	1			26	15	2		23	18	8	
	21	18	10				27		10	7			21	21	3			22	15	14		22	17	12
	29	5	0				26		11	9			21	15	15			21	20	8	8	30	3	3
	29	4	3				23		18	5			19	19	13			20	19	12			26	11
	28	9	1			22	15		13	3*	29		6	4	6		29	8	1			25	17	2
	27	11	4								28		10	3				29	7	4			23	17
	25	15	4								27		10	8				28	11	1		21	21	6
	24	17	1					24	14		11		25	16		5		19	19	14				
	24	13	11	881**	28	9	4		22	20	3		23	19	4									
	23	16	9			26	14	3		21	16	14		23	16	11								
	21	20	5			26	13	6		20	18	13		19	17	16	920*	30	4	2				
	21	19	8			25	16	0	4	29	7	2	7	27	13	3			28	10	6			
	21	16	13			24	17	4			26	13		7		21		21	5		26	12	10	
	19	19	12			22	19	6			25	13		10	8	30		2	2		22	20	6	
	29	5	1			20	20	9			23	19		2			26	14	6		20	18	14	
	25	11	11			20	16	15		23	14	13	9	22		18	10	1	29	8	4			
	23	17	7			19	18	14		22	19	7				30	3		0		28	11	4	
23	13	13	2		29	5	4		22	17	11			29	8	2			26	14	7			
17	17	17			28	7	7	6*	24	16	8			28	11	2			25	14	10			
24	16	6			27	12	3		7	28	8	7		28	10	5		23	14	14				
20	18	12			25	16	1				26	14	5		27	12	6		20	20	11			
9	28	9	2		24	15	9				26	11	10		26	13	8	2	29	9	0			
	28	7	6		23	17	8			25	16	4		24	18	3			27	12	7			
	26	12	7		21	21	0	8	27	13	0		22	20	5		24		15	11				
	25	12	10		20	19	11			27	12	5		22	19	8			21	20	9			
24	17	2	3	21	21	1			23	15	12		22	16	13	3	21	16	15					
23	18	4			21	19	9			21	21	4		21	18		12		29	9	1			
23	14	12		4	28	10	0	9	29	7	3							27	13	5				
18	17	16				28	8		6		27	13	1							25	17	3		
					26	12	8			27	11	7	910	30	3	1		23	15	13				
					22	20	0			25	15	7			27	10	9	5*	21	19	11			
870	29	5	2		22	16	12		23	19	3			26	15	3			30	5	0			
	26	13	5	5	28	10	1		23	17	9			19	18	15			30	4	3			
	25	14	7			25	16	2		21	17	13		28	8	8			27	14	0			
	22	19	5			25	14	8					2*	20	16	16		24	18	5				
2*	26	14	0			23	16	10	900	30	0	0	3	30	3	2	6	22	21	0				
	24	14	10		22	20	1			28	10	4			29	6		6		30	5	1		
	22	18	8		20	17	14			24	18	0			25	12		12		29	9	2		
3	29	4	4		27	11	6			22	20	4			24	16		9		29	7	6		
	28	8	5	6	29	6	3		20	20	10	4	29	8	3		27	14	1					
	27	12	0			25	15	6		28	11		3		26	15	5		26	15	5			
	26	14	1			21	21	2	1	30	1		0		28	9	7		26	13	9			
22	17	10			21	18	11			28	9		6		27	13	4		23	19	6			
19	16	16	8*	28	10	2		26		15	0		27	11	8		22	21	1					
18	18	15			26	14	4			26	12	9		25	17	0		22	19	9				
4	28	9		3		22	20	2		24	18	1		25	15	8		21	17	14				
	27	12		1	9	27	12	4		24	17	6		24	17	7	8*	28	12	0				
	27	9	8			24	13	12	2	30	1	1		24	13	13		9	30	5	2			
	24	17	3			23	18	6			29	6	5		20	17			15		28	12	1	
21	17	12		22		18	9			27	13	2	5	29	7	5				28	9	8		
5	29	5	3							26	15	1			25	17	1			27	14	2		
	27	11	5						25	14	9			25	13	11		27	10	10				
	25	15	5	890	29	7	0		23	18	7			23	19	5	6	24	17	8				
	25	13	9			25	16	3		21	19	10		30	4	0			23	20	0			
23	15	11			25	12	11		18	17	17		24	18	4			23	16	12				
19	17	15			24	17	5	4*	30	2	0		24	14	12			22	21	2				
6	26	14	2		23	19	0			24	18	2						22	18	11				
	22	14	14		21	20	7			18	18	16												

TABLE 3.8.6A (continued)

 $s = h^2 + k^2 + l^2$, \sqrt{s} and mantissa of $\log s$, for $s = 8n + p \not\equiv 4^m \cdot 7 \pmod{4^m \cdot 8}$, $m = 0, 1, 2, \dots$

$n \backslash p$	0	1	2	3	4	5	6
110		881 29·6816 944 976	882 29·6985 945 469	883 29·7153 945 961	884 29·7321 946 452	885 29·7489 946 943	886 29·7658 947 434
111	888 29·7993 948 413	889 29·8161 948 902	890 29·8329 949 390	891 29·8496 949 878		893 29·8831 950 851	894 29·8998 951 338
112	896 29·9333 952 308	897 29·9500 952 792	898 29·9666 953 276	899 29·9833 953 760	900 30·0000 954 243	901 30·0167 954 725	902 30·0333 955 207
113	904 30·0666 956 168	905 30·0832 956 649	906 30·0998 957 128	907 30·1164 957 607	908 30·1330 958 086	909 30·1496 958 564	910 30·1662 959 041
114	912 30·1993 959 995	913 30·2159 960 471	914 30·2324 960 946	915 30·2490 961 421	916 30·2655 961 895	917 30·2820 962 369	918 30·2985 962 843
115	920 30·3315 963 788	921 30·3480 964 260	922 30·3645 964 731	923 30·3809 965 202		925 30·4138 966 142	926 30·4302 966 611
116	928 30·4631 967 548	929 30·4795 968 016	930 30·4959 968 483	931 30·5123 968 950	932 30·5287 969 416	933 30·5450 969 882	934 30·5614 970 347
117	936 30·5941 971 276	937 30·6105 971 740	938 30·6268 972 203	939 30·6431 972 666	940 30·6594 973 128	941 30·6757 973 590	942 30·6920 974 051
118	944 30·7246 974 972	945 30·7409 975 432	946 30·7571 975 891	947 30·7734 976 350	948 30·7896 976 808	949 30·8058 977 266	950 30·8221 977 724
119	952 30·8545 978 637	953 30·8707 979 093	954 30·8869 979 548	955 30·9031 980 003		957 30·9354 980 912	958 30·9516 981 366
120		961 31·0000 982 723	962 31·0161 983 175	963 31·0322 983 626	964 31·0483 984 077	965 31·0644 984 527	966 31·0805 984 977

TABLE 3.8.6A (continued)

Every s followed by all possible (hkl) triplets

s	h	k	l	s	h	k	l	s	h	k	l	s	h	k	l	s	h	k	l
930	29	8	5	942	29	10	1	957*	29	10	4	969	31	2	2	981	31	4	2
	28	11	5		25	14	11		28	13	2		29	8	8		30	9	0
	25	17	4		22	17	13		26	16	5		28	13	4		28	14	1
	25	16	7	4*	28	12	4		20	19	14		28	11	8		26	17	4
	23	20	1		20	20	12	8	30	7	3		26	17	2		26	16	7
	20	19	13	5	30	6	3		29	9	6		22	22	1		25	16	10
1	29	9	3		29	10	2		27	15	2		22	17	14		24	18	9
	27	11	9		26	13	10		25	18	3		20	20	13		23	16	14
	25	15	9		25	16	8					970	31	3	0	2	30	9	1
	21	21	7		24	15	12						27	15	4		26	15	9
2	30	4	4		23	20	4	961**	31	0	0		24	15	13		21	21	10
	28	12	2		22	19	10		30	6	5		23	21	0	4*	28	14	2
	26	16	0		20	17	16		27	14	6		31	3	1		28	10	10
	24	16	10	6	28	9	9		22	21	6	1	29	11	3		22	22	4
3	28	10	7		24	19	3		21	18	14		29	9	7		22	20	10
	26	16	1		24	17	9	2	31	1	0		27	11	11	5	30	9	2
	23	20	2		21	21	8		29	11	0		25	15	11		30	7	6
	22	20	7		21	19	12		28	13	3		23	21	1		29	12	0
4	30	5	3	7	29	9	5		27	13	8		23	19	9		27	16	0
	27	14	3		27	13	7		25	16	9		21	19	13		25	18	6
	27	13	6		19	19	15		24	19	5		30	6	6		24	20	3
	23	18	9	8	28	10	8		23	17	12	2	26	14	10		21	20	12
	22	21	3		26	16	4		21	20	11		22	22	2	6	31	5	0
	22	15	15		22	20	8	3	31	1	1		18	18	18		31	4	3
	21	18	13	9	30	7	0		29	11	1		30	8	3		29	12	1
6*	30	6	0		25	18	0		27	15	3	3	27	12	10		29	9	8
	26	16	2		24	18	7		25	17	7		24	19	6		28	11	9
	26	14	8		20	18	15		25	13	13		31	3	2		27	16	1
	24	18	6						21	21	9	4	30	7	5		25	19	0
	22	16	14						30	8	0		27	14	7		24	19	7
7	30	6	1	950	30	7	1	4	28	12	6		26	17	3		24	17	11
	28	12	3		30	5	5		26	12	12		25	18	5		23	21	4
	27	12	8		29	10	3		24	18	8		23	21	2		21	17	16
	26	15	6		27	14	5	5	31	2	0		19	18	17	7	31	5	1
	24	19	0		27	11	10		30	8	1		22	21	7		29	11	5
	18	18	17		26	15	7		30	7	4		24	20	0		25	19	1
8	29	9	4		25	18	1		28	10	9		24	16	12		23	17	13
	25	13	12		25	17	6		26	17	0	6*	31	4	0		30	8	5
	24	19	1		25	15	10		26	15	8		29	10	6	9*	29	12	2
	23	20	3		23	15	14		25	18	4		28	12	7		28	14	3
9	29	7	7		22	21	5		24	17	10		24	20	1		28	13	6
	25	17	5	2*	30	6	4		23	20	6		22	22	3		27	16	2
	23	19	7		22	18	12		22	20	9		22	18	13		27	14	8
	23	17	11	3	30	7	2		22	16	15		31	4	1		26	13	12
	19	17	17		28	13	0		31	2	1	8	29	11	4		22	21	8
					28	12	5		29	11	2		28	13	5		22	19	12
					26	14	9		29	10	5		25	17	8				
					24	19	4		26	17	1		23	20	7				
					24	16	11		26	13	11		20	17	17	990	31	5	2
940	30	6	2		23	18	10		22	19	11		19	19	16		30	9	3
1	30	5	4		21	16	16		30	8	2		31	3	3		29	10	7
	29	10	0	4	29	8	7		26	16	6	9	27	15	5		27	15	6
	29	8	6		28	13	1		24	14	14		27	13	9		26	17	5
	28	11	6		28	11	7		22	22	0		23	21	3		25	19	2
	27	14	4		27	15	0						23	15	15		25	14	13
	26	16	3		27	12	9										23	19	10
	26	12	11		23	20	5										21	18	15
	24	19	2		23	19	8										28	12	8
	24	14	13		23	16	13										24	20	4
	22	21	4		27	15	1												
	21	20	10	5	21	17	15												
	19	18	16																

TABLE 3.8.6A (continued)

 $s = h^2 + k^2 + l^2$, \sqrt{s} and mantissa of $\log s$, for $s = 8n + p \not\equiv 4^m \cdot 7 \pmod{4^m \cdot 8}$, $m = 0, 1, 2, \dots$

$\begin{matrix} p \\ n \end{matrix}$	0	1	2	3	4	5	6
121	968 31.1127 985 875	969 31.1288 986 324	970 31.1448 986 772	971 31.1609 987 219	972 31.1769 987 666	973 31.1929 988 113	974 31.2090 988 559
122	976 31.2410 989 450	977 31.2570 989 895	978 31.2730 990 339	979 31.2890 990 783	980 31.3050 991 226	981 31.3209 991 669	982 31.3369 992 111
123	984 31.3688 992 995	985 31.3847 993 436	986 31.4006 993 877	987 31.4166 994 317		989 31.4484 995 196	990 31.4643 995 635
124	992 31.4960 996 512	993 31.5119 996 949	994 31.5278 997 386	995 31.5436 997 823	996 31.5595 998 259	997 31.5753 998 695	998 31.5911 999 131

TABLE 3.8.6A (continued)

Every s followed by all possible (hkl) triplets

s	h	k	l
993	31	4	4
	26	14	11
	23	20	8
	22	22	5
4	29	12	3
	27	16	3
	27	12	11
	25	15	12
5	31	5	3
	25	19	3
	25	17	9
	23	21	5
6	28	14	4
	26	16	8
	22	16	16
	20	20	14
7	31	6	0
	30	9	4
	24	15	14
	23	18	12
8	31	6	1
	30	7	7
	29	11	6
	27	13	10
	25	18	7
	22	17	15
	21	19	14

TABLE 3.8.6B
Space Groups in Each of the 17 Cubic Aspects

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
$P \dots$	$P4_2 \dots$	$P4_1 \dots$	$Pn \dots$	$P \dots n$	$Pn \dots n$	$Pa \dots$	$I \dots$	$I4_1 \dots$	$Ia \dots$	$I \dots d$	$Ia \dots d$	$F \dots$	$F4_1 \dots$	$Fd \dots$	$F \dots c$	$Fd \dots c$
$Pm3m$			$Pn3m$	$Pm3n$	$Pn3n$		$Im3m$				$Ia3d$	$Fm3m$		$Fd3m$	$Fm3c$	$Fd3c$
$P432$	$P4_232$	$\begin{cases} P4_132 \\ P4_332 \end{cases}$					$I432$	$I4_132$				$F432$	$F4_132$			
$P\bar{4}3m$				$P\bar{4}3n$			$I\bar{4}3m$			$I\bar{4}3d$		$F\bar{4}3m$			$F\bar{4}3c$	
$Pm3$			$Pn3$			$Pa3$	$Im3$	$Ia3$				$Fm3$		$Fd3$		
$P23$	$P2_13$						$\begin{cases} I23 \\ I2_13 \end{cases}$					$F23$				

TABLE 3.8.6C
Reflections Permitted by Each of the 17 Cubic Aspects
 $s = h^2 + k^2 + l^2$

s	$h k l$ ($h > k > l$)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	$h k l$ ($h < k < l$)	s
		$P \dots$	$P4_2 \dots$	$P4_1 \dots$	$Pn \dots$	$P \dots n$	$Pn \dots n$	$Pa \dots$	$I \dots$	$I4_1 \dots$	$Ia \dots$	$I \dots d$	$Ia \dots d$	$F \dots$	$F4_1 \dots$	$Fd \dots$	$F \dots c$	$Fd \dots c$		
1	1 0 0	+	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	0 0 1	1
2	1 1 0	+	+	+	+	+	+	—	+	+	—	—	—	—	—	—	—	—	0 1 1	2
3	1 1 1	+	+	+	+	—	—	+	—	—	—	—	—	+	+	+	—	—	1 1 1	3
4	2 0 0	+	+	—	+	+	+	+	+	—	+	—	—	+	—	—	+	—	0 0 2	4
5	2 1 0	+	+	+	—	+	—	×	—	—	—	—	—	—	—	—	—	—	0 1 2	5
6	2 1 1	+	+	+	+	+	+	+	+	+	+	+	+	—	—	—	—	—	1 1 2	6
8	2 2 0	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	0 2 2	8
9	$\begin{cases} 3 0 0 \\ 2 2 1 \end{cases}$	+	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	$\begin{cases} 0 0 3 \\ 1 2 2 \end{cases}$	9
10	3 1 0	+	+	+	+	+	+	—	+	+	—	+	—	—	—	—	—	—	0 1 3	10
11	3 1 1	+	+	+	+	—	—	+	—	—	—	—	—	+	+	+	—	—	1 1 3	11
12	2 2 2	+	+	+	+	+	+	+	+	+	+	—	—	+	+	+	+	+	2 2 2	12
13	3 2 0	+	+	+	—	+	—	×	—	—	—	—	—	—	—	—	—	—	0 2 3	13
14	3 2 1	+	+	+	+	+	+	+	+	+	+	+	+	—	—	—	—	—	1 2 3	14
16	4 0 0	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	0 0 4	16
17	$\begin{cases} 4 1 0 \\ 3 2 2 \end{cases}$	+	+	+	—	+	—	×	—	—	—	—	—	—	—	—	—	—	$\begin{cases} 0 1 4 \\ 2 2 3 \end{cases}$	17
18	$\begin{cases} 4 1 1 \\ 3 3 0 \end{cases}$	+	+	+	+	+	+	+	+	+	—	—	—	—	—	—	—	—	$\begin{cases} 1 1 4 \\ 0 3 3 \end{cases}$	18
19	3 3 1	+	+	+	+	—	—	+	—	—	—	—	—	+	+	+	—	—	1 3 3	19
20	4 2 0	+	+	+	+	+	+	+	+	+	+	+	+	+	+	—	+	—	0 2 4	20
21	4 2 1	+	+	+	+	+	+	+	—	—	—	—	—	—	—	—	—	—	1 2 4	21
22	3 3 2	+	+	+	+	+	+	+	+	+	+	+	+	—	—	—	—	—	2 3 3	22
24	4 2 2	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	2 2 4	24
25	$\begin{cases} 5 0 0 \\ 4 3 0 \end{cases}$	+	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	$\begin{cases} 0 0 5 \\ 0 3 4 \end{cases}$	25
26	$\begin{cases} 5 1 0 \\ 4 3 1 \end{cases}$	+	+	+	+	+	+	—	+	+	—	+	—	—	—	—	—	—	$\begin{cases} 0 1 5 \\ 1 3 4 \end{cases}$	26
27	$\begin{cases} 5 1 1 \\ 3 3 3 \end{cases}$	+	+	+	+	—	—	+	—	—	—	—	—	+	+	+	—	—	$\begin{cases} 1 1 5 \\ 3 3 3 \end{cases}$	27
29	$\begin{cases} 5 2 0 \\ 4 3 2 \end{cases}$	+	+	+	—	+	—	×	—	—	—	—	—	—	—	—	—	—	$\begin{cases} 0 2 5 \\ 2 3 4 \end{cases}$	29
30	5 2 1	+	+	+	+	+	+	+	+	+	+	+	+	—	—	—	—	—	1 2 5	30
32	4 4 0	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	0 4 4	32
33	$\begin{cases} 5 2 2 \\ 4 4 1 \end{cases}$	+	+	+	+	—	—	+	—	—	—	—	—	—	—	—	—	—	$\begin{cases} 2 2 5 \\ 1 4 4 \end{cases}$	33

+ indicates presence of reflection. — indicates absence of reflection. * indicates that preceding number is not sum of three squares.
 × indicates that only half of the planes contribute, viz. ($hk0$), ($0hk$), ($k0h$) with h even.

TABLE 3.8.6C (continued)

<i>s</i>	<i>h k l</i> (<i>h</i> > <i>k</i> > <i>l</i>)	1 <i>P...</i>	2 <i>P4₂..</i>	3 <i>P4₁..</i>	4 <i>Pn..</i>	5 <i>P..n</i>	6 <i>Pn.n</i>	7 <i>Pa.</i>	8 <i>I...</i>	9 <i>I4₁..</i>	10 <i>Ia.</i>	11 <i>I..d</i>	12 <i>Ia.d</i>	13 <i>F...</i>	14 <i>F4₁..</i>	15 <i>Fd..</i>	16 <i>F..c</i>	17 <i>Fd.c</i>	<i>h k l</i> (<i>h</i> < <i>k</i> < <i>l</i>)	<i>s</i>
34	{5 3 0 4 3 3	+	+	+	+	+	+	—	+	+	—	+	—	—	—	—	—	—	0 3 5 3 3 4	34
35	5 3 1	+	+	+	+	+	+	+	—	—	—	—	—	+	+	+	+	+	1 3 5	35
36	{6 0 0 4 4 2	+	+	—	+	+	+	+	+	—	+	—	—	+	—	—	+	—	0 0 6 2 4 4	36
37	6 1 0	+	+	+	—	+	—	×	—	—	—	—	—	—	—	—	—	—	0 1 6	37
38	{6 1 1 5 3 2	+	+	+	+	+	+	+	+	+	+	+	+	—	—	—	—	—	1 1 6 2 3 5	38
40	6 2 0	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	0 2 6	40
41	{6 2 1 5 4 0 4 4 3	+	+	+	+	+	+	+	—	—	—	—	—	—	—	—	—	—	1 2 6 0 4 5 3 4 4	41
42	5 4 1	+	+	+	+	+	+	+	+	+	+	+	+	—	—	—	—	—	1 4 5	42
43	5 3 3	+	+	+	+	—	—	+	—	—	—	—	—	+	+	+	—	—	3 3 5	43
44	6 2 2	+	+	+	+	+	+	+	+	+	—	—	—	+	+	+	+	+	2 2 6	44
45	{6 3 0 5 4 2	+	+	+	—	+	—	×	—	—	—	—	—	—	—	—	—	—	0 3 6 2 4 5	45
46	6 3 1	+	+	+	+	+	+	+	+	+	+	+	+	—	—	—	—	—	1 3 6	46
48	4 4 4	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	4 4 4	48
49	{7 0 0 6 3 2 7 1 0	+	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	0 0 7 2 3 6 0 1 7	49
50	{5 5 0 5 4 3	+	+	+	+	+	+	—	+	+	—	—	—	—	—	—	—	—	0 5 5 3 4 5	50
51	{7 1 1 5 5 1	+	+	+	+	—	—	+	—	—	—	—	—	+	+	+	—	—	1 1 7 1 5 5	51
52	6 4 0	+	+	+	+	+	+	+	+	+	+	+	+	+	+	—	+	—	0 4 6	52
53	{7 2 0 6 4 1 7 2 1	+	+	+	—	+	—	×	—	—	—	—	—	—	—	—	—	—	0 2 7 1 4 6 1 2 7	53
54	{6 3 3 5 5 2	+	+	+	+	+	+	+	+	+	+	+	+	—	—	—	—	—	3 3 6 2 5 5	54
56	6 4 2	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	2 4 6	56
57	{7 2 2 5 4 4	+	+	+	+	—	—	+	—	—	—	—	—	—	—	—	—	—	2 2 7 4 4 5	57
58	7 3 0	+	+	+	+	+	+	—	+	+	—	+	—	—	—	—	—	—	0 3 7	58
59	{7 3 1 5 5 3	+	+	+	+	+	+	+	—	—	—	—	—	+	+	+	+	+	1 3 7 3 5 5	59
61	{6 5 0 6 4 3	+	+	+	—	+	—	×	—	—	—	—	—	—	—	—	—	—	0 5 6 3 4 6	61
62	{7 3 2 6 5 1	+	+	+	+	+	+	+	+	+	+	+	+	—	—	—	—	—	2 3 7 1 5 6	62
64	8 0 0	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	0 0 8	64
65	{8 1 0 7 4 0 6 5 2	+	+	+	—	+	—	×	—	—	—	—	—	—	—	—	—	—	0 1 8 0 4 7 2 5 6	65
66	{8 1 1 7 4 1 5 5 4	+	+	+	+	+	+	+	+	+	+	—	—	—	—	—	—	—	1 1 8 1 4 7 4 5 5	66
67	7 3 3	+	+	+	+	—	—	+	—	—	—	—	—	+	+	+	—	—	3 3 7	67
68	{8 2 0 6 4 4	+	+	+	+	+	+	+	+	+	+	+	+	+	+	—	+	—	0 2 8 4 4 6	68

+ indicates presence of reflection. — indicates absence of reflection. * indicates that preceding number is not sum of three squares.
 × indicates that only half of the planes contribute, viz. (*hk*0), (*Ohk*), (*k*0*h*) with *h* even.

TABLE 3.8.6C (continued)

<i>s</i>	<i>h k l</i> (<i>h</i> > <i>k</i> > <i>l</i>)	1 <i>P...</i>	2 <i>P4₂..</i>	3 <i>P4₁..</i>	4 <i>Pn..</i>	5 <i>P..n</i>	6 <i>Pn.n</i>	7 <i>Pa.</i>	8 <i>I...</i>	9 <i>I4₁..</i>	10 <i>Ia.</i>	11 <i>I..d</i>	12 <i>Ia.d</i>	13 <i>F...</i>	14 <i>F4₁..</i>	15 <i>Fd..</i>	16 <i>F..c</i>	17 <i>Fd.c</i>	<i>h k l</i> (<i>h</i> < <i>k</i> < <i>l</i>)	<i>s</i>
69	{8 2 1 7 4 2}	+	+	+	+	+	+	+	—	—	—	—	—	—	—	—	—	—	1 2 8 2 4 7	69
70	6 5 3	+	+	+	+	+	+	+	+	+	+	+	+	—	—	—	—	—	3 5 6	70
72	{8 2 2 6 6 0}	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	2 2 8 0 6 6	72
73	{8 3 0 6 6 1}	+	+	+	—	+	—	×	—	—	—	—	—	—	—	—	—	—	0 3 8 1 6 6	73
74	{8 3 1 7 5 0 7 4 3}	+	+	+	+	+	+	+	+	+	+	+	+	—	—	—	—	—	1 3 8 0 5 7 3 4 7	74
75	{7 5 1 5 5 5}	+	+	+	+	+	+	+	—	—	—	—	—	+	+	+	+	+	1 5 7 5 5 5	75
76	6 6 2	+	+	+	+	+	+	+	+	+	—	—	—	+	+	+	+	+	2 6 6	76
77	{8 3 2 6 5 4}	+	+	+	+	+	+	+	—	—	—	—	—	—	—	—	—	—	2 3 8 4 5 6	77
78	7 5 2	+	+	+	+	+	+	+	+	+	+	+	+	—	—	—	—	—	2 5 7	78
80	8 4 0	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	0 4 8	80
81	{9 0 0 8 4 1 7 4 4 6 6 3}	+	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	—	0 0 9 1 4 8 4 4 7 3 6 6	81
82	{9 1 0 8 3 3}	+	+	+	+	+	+	—	+	+	—	+	—	—	—	—	—	—	0 1 9 3 3 8	82
83	{9 1 1 7 5 3}	+	+	+	+	—	—	+	—	—	—	—	—	+	+	+	—	—	1 1 9 3 5 7	83
84	8 4 2	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	2 4 8	84
85	{9 2 0 7 6 0}	+	+	+	—	+	—	×	—	—	—	—	—	—	—	—	—	—	0 2 9 0 6 7	85
86	{9 2 1 7 6 1 6 5 5}	+	+	+	+	+	+	+	+	+	+	+	+	—	—	—	—	—	1 2 9 1 6 7 5 5 6	86
88	6 6 4	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	4 6 6	88
89	{9 2 2 8 5 0 8 4 3 7 6 2}	+	+	+	+	—	—	+	—	—	—	—	—	—	—	—	—	—	2 2 9 0 5 8 3 4 8 2 6 7	89
90	{9 3 0 8 5 1 7 5 4}	+	+	+	+	+	+	—	+	+	—	+	—	—	—	—	—	—	0 3 9 1 5 8 4 5 7	90
91	9 3 1	+	+	+	+	+	+	+	—	—	—	—	—	+	+	+	+	+	1 3 9	91
93	8 5 2	+	+	+	+	+	+	+	—	—	—	—	—	—	—	—	—	—	2 5 8	93
94	{9 3 2 7 6 3}	+	+	+	+	+	+	+	+	+	+	+	+	—	—	—	—	—	2 3 9 3 6 7	94
96	8 4 4	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	4 4 8	96
97	{9 4 0 6 6 5}	+	+	+	—	+	—	×	—	—	—	—	—	—	—	—	—	—	0 4 9 5 6 6	97
98	{9 4 1 8 5 3 7 7 0}	+	+	+	+	+	+	+	+	+	+	+	+	—	—	—	—	—	1 4 9 3 5 8 0 7 7	9
99	{9 3 3 7 7 1 7 5 5}	+	+	+	+	—	—	+	—	—	—	—	—	+	+	+	—	—	3 3 9 1 7 7 5 5 7	99
100	{10 0 0 8 6 0}	+	+	+	+	+	+	+	+	—	+	—	—	+	—	—	+	—	0 0 10 0 6 8	100

+ indicates presence of reflection. — indicates absence of reflection. * indicates that preceding number is not sum of three squares.
 × indicates that only half of the planes contribute, viz. (*hk*0), (0*hk*), (*k*0*h*) with *h* even.

3.9. Hexagonal-rhombohedral Transformations*

3.9.1. Transformation of Cell Constants

The following symbols are used (see stereographic projection, Fig. 3.9.1):

- a, c : edges of the hexagonal cell
- a_R : edge of the rhombohedral cell
- α : angle between the rhombohedral axes
- α' : supplement of α ($\alpha' = 180^\circ - \alpha$)
- ρ_1 : interfacial angle (0001:10 $\bar{1}$ 1)
- ρ_2 : interfacial angle (0001:01 $\bar{1}$ 2)
- λ : interfacial angle (10 $\bar{1}$ 1: $\bar{1}$ 101)

The quantities given in Table 3.9.1 were calculated by means of the following relations:

$$\begin{aligned}\tan \rho_2 &= \frac{1}{2} \tan \rho_1 \\ \frac{c}{a} &= \frac{\sqrt{3}}{2} \tan \rho_1 \\ \cos \frac{\alpha'}{2} &= \frac{\sqrt{3}}{2} \cos \rho_2 \\ \sin \frac{\lambda}{2} &= \frac{\sqrt{3}}{2} \sin \rho_1 \\ \frac{a_R}{a} &= \frac{1}{\sqrt{3} \cos \rho_2}\end{aligned}$$

On the chart (Fig. 3.9.1) angles and ratios are plotted as functions of ρ_1 .

3.9.2. Transformation of Indices

From the two possible rhombohedral settings (Vol. I, p. 20) the obverse has been selected for use in Table

3.9.2. The obverse rhombohedral axes in terms of the hexagonal axes (Vol. I, Table 2.5.1, p. 21) are given by:

$$a_R = \frac{2}{3}a + \frac{1}{3}b + \frac{1}{3}c, \quad b_R = -\frac{1}{3}a + \frac{1}{3}b + \frac{1}{3}c, \quad c_R = -\frac{1}{3}a - \frac{2}{3}b + \frac{1}{3}c$$

The rhombohedral indices in terms of the hexagonal indices likewise are expressed:

$$h_R = \frac{1}{3}(2h+k+l), \quad k_R = \frac{1}{3}(-h+k+l), \quad l_R = \frac{1}{3}(-h-2k+l)$$

The rhombohedral criterion takes the form “ $(-h+k+l)$ divisible by 3.” Table 3.9.2 consists of one column of hexagonal indices $hkil_0$ ($l_0=0, 1$ or 2) obeying the criterion, for successive positive h, k values up to $h+k=20$; and a second column of corresponding rhombohedral indices $h_R k_R l_R$. Given $hkil$ where $l=3n+l_0$, the corresponding rhombohedral indices will be h_R+n, k_R+n, l_R+n .

EXAMPLE. To transform (2.1. $\bar{3}$.13) to rhombohedral indices, note that $13=3n+l_0$, where $l_0=1, n=4$. Next to (21 $\bar{3}$ 1), Table 3.9.2 gives (20 $\bar{1}$). Hence the desired rhombohedral indices will be (2+4, 0+4, $\bar{1}$ +4); and (2.1. $\bar{3}$.13) becomes (643).

The transformation of rhombohedral to hexagonal indices is best carried out directly by means of the relations

$$h=h_R-k_R, \quad k=k_R-l_R, \quad i=l_R-h_R, \quad l=h_R+k_R+l_R$$

Transformation of hexagonal indices $hkil$ to ortho-hexagonal indices $h_0 k_0 l_0$ can also be done by inspection. For example, if the setting O_1 (Vol. 1, Fig. 2.5.2, p. 19) is used:

$$h_0=h, \quad k_0=h+2k, \quad l_0=l$$

* Section 3.9.1 was contributed by A. Pabst, to whom we are further indebted for many critical comments and suggestions on the whole of Section 3.

3.9. HEXAGONAL-RHOMBOHEDRAL TRANSFORMATIONS

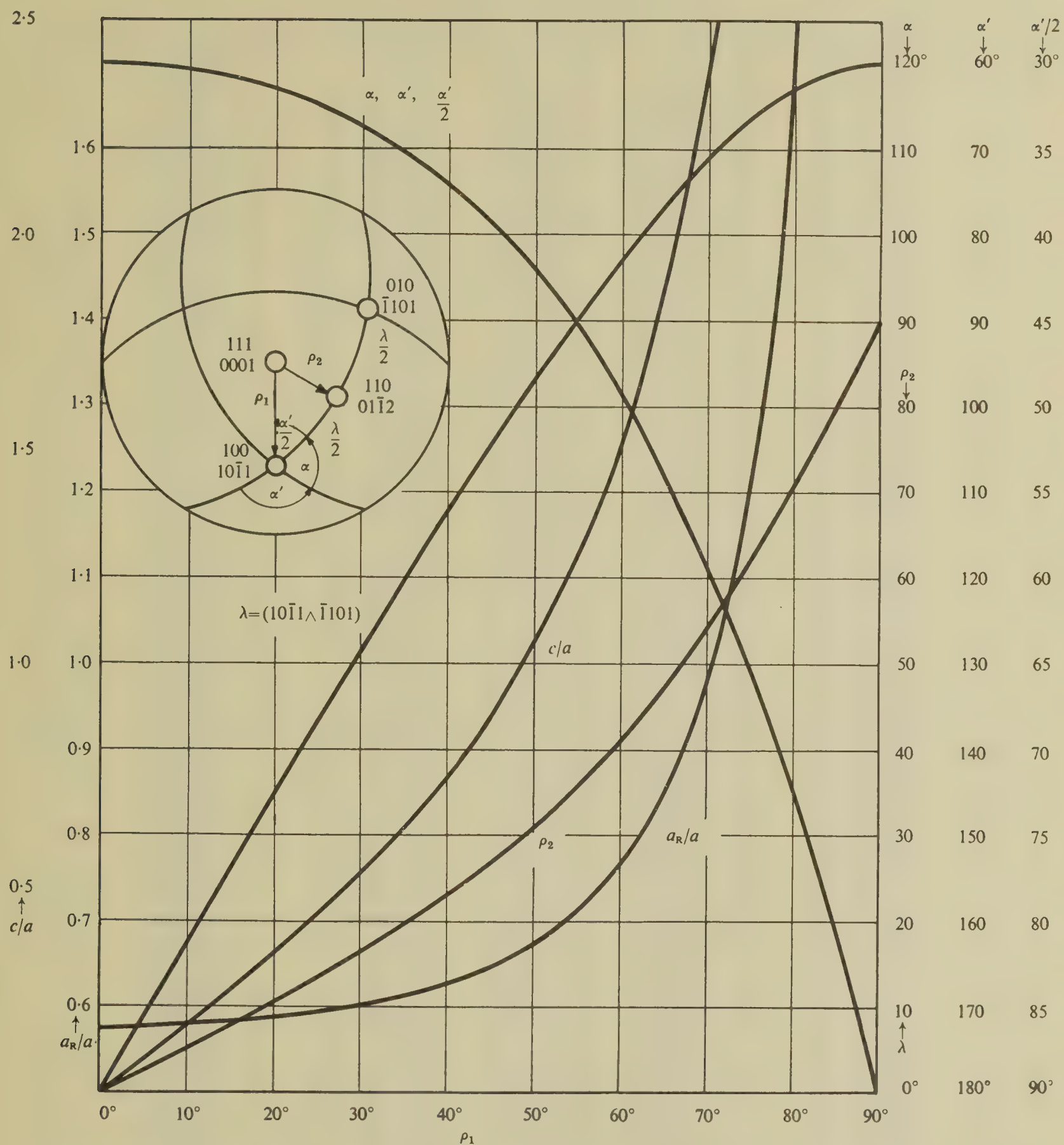


Fig. 3.9.1. Correlation of axial elements and angles of rhombohedral and hexagonal cells.

3.9. HEXAGONAL-RHOMBOHEDRAL TRANSFORMATIONS

TABLE 3.9.1
Hexagonal and Rhombohedral Constants
Contributed by A. Pabst

ρ_1	ρ_2	c/a	α	λ	a_R/a
0°	0° 00'	0.00000	120° 00'	0° 00'	0.57735
30'	0 15	0.00756	120 00	0 52	0.57736
1	0 30	0.01512	119 59½	1 44	0.57737
30	0 45	0.02268	119 59	2 36	0.57740
2	1 00	0.03024	119 58	3 28	0.57744
30	1 15	0.03781	119 57	4 20	0.57749
3	1 30	0.04539	119 56	5 12	0.57755
30	1 45	0.05297	119 54½	6 3½	0.57762
4	2 00	0.06056	119 53	6 55½	0.57770
30	2 15	0.06816	119 51	7 47½	0.57779
5	2 30½	0.07577	119 49	8 39½	0.57790
30	2 45½	0.08339	119 46	9 31½	0.57801
6	3 00½	0.09102	119 44	10 23½	0.57815
30	3 15½	0.09867	119 41	11 15	0.57828
7	3 31	0.10633	119 38	12 7	0.57844
30	3 46	0.11401	119 34	12 59	0.57860
8	4 1	0.12171	119 31	13 50½	0.57877
30	4 16½	0.12943	119 27	14 42½	0.57896
9	4 31½	0.13716	119 23	15 34	0.57916
30	4 47	0.14492	119 19	16 26	0.57936
10	5 2½	0.15270	119 14	17 18	0.57959
30	5 17½	0.16051	119 9½	18 10	0.57982
11	5 33	0.16834	119 4½	19 1½	0.58007
30	5 48½	0.17619	118 59½	19 53	0.58033
12	6 4	0.18408	118 54	20 45	0.58060
30	6 19½	0.19199	118 48	21 36½	0.58088
13	6 35	0.19994	118 42	22 28	0.58118
30	6 50½	0.20791	118 36	23 19½	0.58149
14	7 6½	0.21593	118 29½	24 11½	0.58182
30	7 22	0.22397	118 23	25 3	0.58215
15	7 38	0.23205	118 16	25 54½	0.58251
30	7 53½	0.24017	118 8½	26 46	0.58287
16	8 9½	0.24833	118 1	27 37½	0.58325
30	8 25½	0.25653	117 53½	28 29	0.58364
17	8 41½	0.26477	117 46	29 20	0.58406
30	8 57½	0.27306	117 37½	30 11½	0.58448
18	9 13½	0.28139	117 29	31 3	0.58492
30	9 30	0.28977	117 20	31 54	0.58537
19	9 46	0.29820	117 11	32 45	0.58584
30	10 2½	0.30668	117 2	33 36½	0.58632
20	10 19	0.31521	116 52	34 27½	0.58683
30	10 35½	0.32379	116 42	35 18½	0.58735
21	10 52	0.33243	116 32	36 10	0.58789
30	11 8½	0.34114	116 21½	37 1	0.58844
22	11 25	0.34990	116 10½	37 51½	0.58901
30	11 42	0.35872	116 00	38 42½	0.58960
23	11 59	0.36760	115 48½	39 33½	0.59021
30	12 16	0.37656	115 37	40 24	0.59084
24	12 33	0.38558	115 25	41 15	0.59148
30	12 50	0.39467	115 13	42 5½	0.59215
25	13 7½	0.40384	115 00	42 56	0.59284

3.9. HEXAGONAL-RHOMBOHEDRAL TRANSFORMATIONS

TABLE 3.9.1. (continued)

ρ_1	ρ_2	c/a	α	λ	a_R/a
25°	13° 7½'	0.40384	115° 00'	42° 56'	0.59284
30'	13 25	0.41308	114 47½	43 47	0.59354
26	13 42½	0.42239	114 34	44 37	0.59427
30	14 00	0.43178	114 20½	45 28	0.59502
27	14 17½	0.44127	114 7	46 18	0.59579
30	14 35½	0.45083	113 53	47 8½	0.59659
28	14 53½	0.46047	113 38	47 59	0.59741
30	15 11½	0.47022	113 23½	48 49	0.59825
29	15 29½	0.48005	113 8	49 39	0.59912
30	15 47½	0.48997	112 53	50 29	0.60001
30	16 6	0.50000	112 37½	51 19	0.60092
30	16 24½	0.51013	112 21	52 9	0.60187
31	16 43½	0.52036	112 4½	52 59	0.60284
30	17 2	0.53070	111 47½	53 48½	0.60385
32	17 21	0.54116	111 30½	54 38	0.60487
30	17 40	0.55172	111 13	55 27½	0.60593
33	17 59½	0.56241	110 55	56 17	0.60702
30	18 18½	0.57321	110 36½	57 6½	0.60815
34	18 38	0.58414	110 18	57 56	0.60930
30	18 58	0.59520	109 58½	58 45	0.61049
35	19 17½	0.60640	109 39	59 34	0.61171
30	19 37½	0.61773	109 19	60 23	0.61297
36	19 58	0.62921	108 58	61 12	0.61427
30	20 18	0.64082	108 37½	62 1	0.61560
37	20 38½	0.65260	108 16½	62 49½	0.61697
30	20 59½	0.66453	107 54½	63 38	0.61838
38	21 20½	0.67662	107 32½	64 26½	0.61984
30	21 41½	0.68887	107 10	65 15	0.62134
39	22 2½	0.70129	106 47	66 3	0.62287
30	22 24	0.71389	106 23½	66 51	0.62447
40	22 45½	0.72668	105 59½	67 39	0.62610
30	23 7½	0.73965	105 35	68 27	0.62779
41	23 29½	0.75283	105 10	69 14½	0.62953
30	23 52	0.76620	104 44½	70 2½	0.63132
42	24 14	0.77977	104 18½	70 50	0.63316
30	24 37	0.79356	103 52	71 37	0.63506
43	25 00	0.80759	103 25½	72 24	0.63703
30	25 23	0.82183	102 58	73 11	0.63904
44	25 46½	0.83631	102 30	73 58	0.64114
30	26 10	0.85104	102 1½	74 45	0.64328
45	26 34	0.86603	101 32	75 31	0.64552
30	26 58	0.88127	101 2½	76 18	0.64778
46	27 22½	0.89679	100 32½	77 4	0.65014
30	27 47	0.91260	100 1½	77 50	0.65258
47	28 12	0.92873	99 30	78 36	0.65511
30	28 37	0.94509	98 58	79 21½	0.65771
48	29 2½	0.96182	98 25½	80 7	0.66040
30	29 28½	0.97886	97 52	80 52½	0.66317
49	29 54½	0.99628	97 18	81 37½	0.66605
30	30 20½	1.01394	96 43½	82 22½	0.66900
50	30 47½	1.03213	96 8	83 7½	0.67209
30	31 14½	1.05058	95 32½	83 51½	0.67525
51	31 41½	1.0694	94 56	84 36	0.67854

3.9. HEXAGONAL-RHOMBOHEDRAL TRANSFORMATIONS

TABLE 3.9.1 (continued)

ρ_1	ρ_2	c/a	α	λ	a_R/a	
51°	31° 41½'	1.0694	94° 56'	84° 36'	0.67854	
30'	32 9	1.0888	94 18½	85 20	0.68194	
52	32 37	1.1084	93 41	86 4	0.68546	
30	33 5½	1.1286	93 2	86 48	0.68911	
53	33 34	1.1492	92 22½	87 31½	0.69288	
30	34 3	1.1703	91 42½	88 14½	0.69679	
54	34 32	1.1920	91 2	88 57½	0.70085	
30	35 1½	1.2141	90 20	89 40	0.70506	
54° 44' 8"	35° 15' 52"	1.224745	90° 00' 00"	90° 00' 00"	0.707107	{ Simple cube
55	35 32	1.2368	89 37½	90 22½	0.70943	
30	36 2	1.2601	88 54½	91 4½	0.71397	
56	36 33	1.2840	88 10	91 46½	0.71868	
30	37 4	1.3084	87 25½	92 28	0.72357	
57	37 35½	1.3336	86 39½	93 9	0.72865	
30	38 7½	1.3594	85 53	93 50½	0.73393	
58	38 40	1.3859	85 5½	94 31	0.73943	
30	39 13	1.4133	84 17	95 11½	0.74515	
59	39 46	1.4413	83 28	95 51½	0.75110	
30	40 19½	1.4703	82 38	96 31½	0.75730	
60	40 53½	1.5000	81 47	97 11	0.76376	
30	41 28	1.5307	80 55½	97 50	0.77050	
61	42 3	1.5623	80 2½	98 28½	0.77751	
30	42 38½	1.5950	79 8½	99 7	0.78486	
62	43 14½	1.6287	78 14	99 45	0.79252	
62° 3' 42"	43° 18' 50"	1.6330065	78° 7' 8"	99° 49' 50"	0.7934915	{ Hex. close- packing
30	43 51	1.6636	77 18	100 23	0.80052	
63	44 28	1.6997	76 21	101 00	0.80892	
30	45 5	1.7370	75 23½	101 37	0.81766	
64	45 43	1.7756	74 25	102 13½	0.82683	
30	46 21	1.8156	73 25	102 49½	0.83644	
65	47 00	1.8572	72 24½	103 25	0.84651	
30	47 39	1.9003	71 22½	104 9½	0.85707	
66	48 19	1.9451	70 19½	104 35	0.86818	
30	48 59½	1.9917	69 15½	105 9½	0.87987	
67	49 40	2.0402	68 10½	105 43½	0.89210	
30	50 21½	2.0908	67 4½	106 17	0.90501	
68	51 3½	2.1435	65 57	106 50	0.91860	
30	51 46	2.1985	64 49	107 22	0.93295	
69	52 29	2.2561	63 39½	107 54	0.94809	
30	53 13	2.3163	62 29	108 25½	0.96408	
70	53 57	2.3794	61 17	108 56	0.98101	
30	54 41½	2.4456	60 4½	109 26½	0.99893	
70° 31' 44"	54° 44' 8"	2.4495098	60° 00'	109° 28' 16"	1.0000	{ Cubic close- packing
71	55 27	2.5151	58 50	109 56½	1.0180	
30	56 12½	2.5883	57 35	110 25½	1.0381	
72	56 59	2.6654	56 18½	110 54	1.0596	
30	57 46	2.7467	55 1½	111 22	1.0824	
73	58 33	2.8327	53 43	111 49½	1.1068	

3.9. HEXAGONAL-RHOMBOHEDRAL TRANSFORMATIONS

TABLE 3.9.1 (continued)

ρ_1	ρ_2	c/a	α	λ	a_R/a
73°	58° 33'	2.8327	53° 43'	111° 49½'	1.1068
30'	59 21½	2.9237	52 23	112 16½	1.1327
74	60 10	3.0202	51 2½	112 42½	1.1605
30	60 59	3.1228	49 40½	113 8	1.1903
75	61 49	3.2321	48 17½	113 33	1.2223
30	62 39	3.3487	46 53½	113 57	1.2567
76	63 30	3.4735	45 28	114 20½	1.2939
30	64 21	3.6073	44 2	114 43½	1.3338
77	65 13	3.7512	42 34½	115 5½	1.3772
30	66 5½	3.9064	41 6	115 27	1.4244
78	66 58	4.0743	39 36½	115 48	1.4757
30	67 51½	4.2567	38 6	116 7½	1.5318
79	68 45½	4.4554	36 34½	116 27	1.5934
30	69 39½	4.6727	35 2	116 45½	1.6611
80	70 34½	4.9115	33 28½	117 3½	1.7360
30	71 29½	5.1752	31 54	117 20	1.8192
81	72 25½	5.4679	30 19½	117 36	1.9118
30	73 21½	5.7947	28 43	117 51½	2.0160
82	74 18	6.1621	27 6½	118 6	2.1336
30	75 15	6.5782	25 28½	118 19½	2.2677
83	76 12	7.0532	23 50	118 32	2.4212
30	77 10	7.6010	22 11	118 44	2.5986
84	78 8	8.2397	20 31½	118 55½	2.8066
30	79 6	8.9937	18 51	119 6	3.0531
85	80 4½	9.8987	17 10	119 15	3.3497
30	81 3½	11.004	15 29	119 23½	3.7133
86	82 2½	12.385	13 46½	119 31	4.1686
30	83 1½	14.160	12 4	119 38	4.7551
87	84 1	16.525	10 22½	119 44	5.5381
30	85 0½	19.835	8 38½	119 49	6.6370
88	86 0½	24.800	6 55	119 53	8.2866
30	87 00	33.072	5 11½	119 56	11.039
89	88 00	49.615	3 28	119 58	16.538
30	89 00	99.238	1 44	119 59½	33.177
90	90 00	—	0 00	120 00	—

TABLE 3.9.2

Hexagonal-to-Rhombohedral Transformation of Indices

Given $hkil$, where $l=3n+l_0$, the corresponding rhombohedral indices are h_R+n , k_R+n , l_R+n .

$hkil_0$	$h_R k_R l_R$	$hkil_0$	$h_R k_R l_R$	$hkil_0$	$h_R k_R l_R$
0 1 $\bar{1}$ 2	1 1 0	2 0 $\bar{2}$ 2	2 0 0	4 2 $\bar{6}$ 2	4 0 $\bar{2}$
0 2 $\bar{2}$ 1	1 1 $\bar{1}$	2 1 $\bar{3}$ 1	2 0 $\bar{1}$	4 3 $\bar{7}$ 1	4 0 $\bar{3}$
0 3 $\bar{3}$ 0	1 1 $\bar{2}$	2 2 $\bar{4}$ 0	2 0 $\bar{2}$	4 4 $\bar{8}$ 0	4 0 $\bar{4}$
0 4 $\bar{4}$ 2	2 2 $\bar{2}$	2 3 $\bar{5}$ 2	3 1 $\bar{2}$	4 5 $\bar{9}$ 2	5 1 $\bar{4}$
0 5 $\bar{5}$ 1	2 2 $\bar{3}$	2 4 $\bar{6}$ 1	3 1 $\bar{3}$	4 6 $\bar{10}$ 1	5 1 $\bar{5}$
0 6 $\bar{6}$ 0	2 2 $\bar{4}$	2 5 $\bar{7}$ 0	3 1 $\bar{4}$	4 7 $\bar{11}$ 0	5 1 $\bar{6}$
0 7 $\bar{7}$ 2	3 3 $\bar{4}$	2 6 $\bar{8}$ 2	4 2 $\bar{4}$	4 8 $\bar{12}$ 2	6 2 $\bar{6}$
0 8 $\bar{8}$ 1	3 3 $\bar{5}$	2 7 $\bar{9}$ 1	4 2 $\bar{5}$	4 9 $\bar{13}$ 1	6 2 $\bar{7}$
0 9 $\bar{9}$ 0	3 3 $\bar{6}$	2 8 $\bar{10}$ 0	4 2 $\bar{6}$	4 10 $\bar{14}$ 0	6 2 $\bar{8}$
0 10 $\bar{10}$ 2	4 4 $\bar{6}$	2 9 $\bar{11}$ 2	5 3 $\bar{6}$	4 11 $\bar{15}$ 2	7 3 $\bar{8}$
0 11 $\bar{11}$ 1	4 4 $\bar{7}$	2 10 $\bar{12}$ 1	5 3 $\bar{7}$	4 12 $\bar{16}$ 1	7 3 $\bar{9}$
0 12 $\bar{12}$ 0	4 4 $\bar{8}$	2 11 $\bar{13}$ 0	5 3 $\bar{8}$	4 13 $\bar{17}$ 0	7 3 $\bar{10}$
0 13 $\bar{13}$ 2	5 5 $\bar{8}$	2 12 $\bar{14}$ 2	6 4 $\bar{8}$	4 14 $\bar{18}$ 2	8 4 $\bar{10}$
0 14 $\bar{14}$ 1	5 5 $\bar{9}$	2 13 $\bar{15}$ 1	6 4 $\bar{9}$	4 15 $\bar{19}$ 1	8 4 $\bar{11}$
0 15 $\bar{15}$ 0	5 5 $\bar{10}$	2 14 $\bar{16}$ 0	6 4 $\bar{10}$	4 16 $\bar{20}$ 0	8 4 $\bar{12}$
0 16 $\bar{16}$ 2	6 6 $\bar{10}$	2 15 $\bar{17}$ 2	7 5 $\bar{10}$		
0 17 $\bar{17}$ 1	6 6 $\bar{11}$	2 16 $\bar{18}$ 1	7 5 $\bar{11}$	5 0 $\bar{3}$ 2	4 $\bar{1}$ $\bar{1}$
0 18 $\bar{18}$ 0	6 6 $\bar{12}$	2 17 $\bar{19}$ 0	7 5 $\bar{12}$	5 1 $\bar{6}$ 1	4 $\bar{1}$ $\bar{2}$
0 19 $\bar{19}$ 2	7 7 $\bar{12}$	2 18 $\bar{20}$ 2	8 6 $\bar{12}$	5 2 $\bar{7}$ 0	4 $\bar{1}$ $\bar{3}$
0 20 $\bar{20}$ 1	7 7 $\bar{13}$			5 3 $\bar{8}$ 2	5 0 $\bar{3}$
		3 0 $\bar{3}$ 0	2 $\bar{1}$ $\bar{1}$	5 4 $\bar{9}$ 1	5 0 $\bar{4}$
1 0 $\bar{1}$ 1	1 0 0	3 1 $\bar{4}$ 2	3 0 $\bar{1}$	5 5 $\bar{10}$ 0	5 0 $\bar{5}$
1 1 $\bar{2}$ 0	1 0 $\bar{1}$	3 2 $\bar{5}$ 1	3 0 $\bar{2}$	5 6 $\bar{11}$ 2	6 1 $\bar{5}$
1 2 $\bar{3}$ 2	2 1 $\bar{1}$	3 3 $\bar{6}$ 0	3 0 $\bar{3}$	5 7 $\bar{12}$ 1	6 1 $\bar{6}$
1 3 $\bar{4}$ 1	2 1 $\bar{2}$	3 4 $\bar{7}$ 2	4 1 $\bar{3}$	5 8 $\bar{13}$ 0	6 1 $\bar{7}$
1 4 $\bar{5}$ 0	2 1 $\bar{3}$	3 5 $\bar{8}$ 1	4 1 $\bar{4}$	5 9 $\bar{14}$ 2	7 2 $\bar{7}$
1 5 $\bar{6}$ 2	3 2 $\bar{3}$	3 6 $\bar{9}$ 0	4 1 $\bar{5}$	5 10 $\bar{15}$ 1	7 2 $\bar{8}$
1 6 $\bar{7}$ 1	3 2 $\bar{4}$	3 7 $\bar{10}$ 2	5 2 $\bar{5}$	5 11 $\bar{16}$ 0	7 2 $\bar{9}$
1 7 $\bar{8}$ 0	3 2 $\bar{5}$	3 8 $\bar{11}$ 1	5 2 $\bar{6}$	5 12 $\bar{17}$ 2	8 3 $\bar{9}$
1 8 $\bar{9}$ 2	4 3 $\bar{5}$	3 9 $\bar{12}$ 0	5 2 $\bar{7}$	5 13 $\bar{18}$ 1	8 3 $\bar{10}$
1 9 $\bar{10}$ 1	4 3 $\bar{6}$	3 10 $\bar{13}$ 2	6 3 $\bar{7}$	5 14 $\bar{19}$ 0	8 3 $\bar{11}$
1 10 $\bar{11}$ 0	4 3 $\bar{7}$	3 11 $\bar{14}$ 1	6 3 $\bar{8}$	5 15 $\bar{20}$ 2	9 4 $\bar{11}$
1 11 $\bar{12}$ 2	5 4 $\bar{7}$	3 12 $\bar{15}$ 0	6 3 $\bar{9}$		
1 12 $\bar{13}$ 1	5 4 $\bar{8}$	3 13 $\bar{16}$ 2	7 4 $\bar{9}$	6 0 $\bar{6}$ 0	4 $\bar{2}$ $\bar{2}$
1 13 $\bar{14}$ 0	5 4 $\bar{9}$	3 14 $\bar{17}$ 1	7 4 $\bar{10}$	6 1 $\bar{7}$ 2	5 $\bar{1}$ $\bar{2}$
1 14 $\bar{15}$ 2	6 5 $\bar{9}$	3 15 $\bar{18}$ 0	7 4 $\bar{11}$	6 2 $\bar{8}$ 1	5 $\bar{1}$ $\bar{3}$
1 15 $\bar{16}$ 1	6 5 $\bar{10}$	3 16 $\bar{19}$ 2	8 5 $\bar{11}$	6 3 $\bar{9}$ 0	5 $\bar{1}$ $\bar{4}$
1 16 $\bar{17}$ 0	6 5 $\bar{11}$	3 17 $\bar{20}$ 1	8 5 $\bar{12}$	6 4 $\bar{10}$ 2	6 0 $\bar{4}$
1 17 $\bar{18}$ 2	7 6 $\bar{11}$			6 5 $\bar{11}$ 1	6 0 $\bar{5}$
1 18 $\bar{19}$ 1	7 6 $\bar{12}$	4 0 $\bar{4}$ 1	3 $\bar{1}$ $\bar{1}$	6 6 $\bar{12}$ 0	6 0 $\bar{6}$
1 19 $\bar{20}$ 0	7 6 $\bar{13}$	4 1 $\bar{5}$ 0	3 $\bar{1}$ $\bar{2}$	6 7 $\bar{13}$ 2	7 1 $\bar{6}$

3.9. HEXAGONAL-RHOMBOHEDRAL TRANSFORMATIONS

TABLE 3.9.2 (continued)

$hkil_0$	$h_R k_R l_R$	$hkil_0$	$h_R k_R l_R$	$hkil_0$	$h_R k_R l_R$
6 8 $\overline{14}$ 1	7 1 $\overline{7}$	9 4 $\overline{13}$ 2	8 $\overline{1}$ $\overline{3}$	13 0 $\overline{13}$ 1	9 4 4
6 9 $\overline{15}$ 0	7 1 $\overline{8}$	9 5 $\overline{14}$ 1	8 $\overline{1}$ $\overline{6}$	13 1 $\overline{14}$ 0	9 4 3
6 10 $\overline{16}$ 2	8 2 $\overline{8}$	9 6 $\overline{15}$ 0	8 $\overline{1}$ $\overline{7}$	13 2 $\overline{15}$ 2	10 3 3
6 11 $\overline{17}$ 1	8 2 $\overline{9}$	9 7 $\overline{16}$ 2	9 0 $\overline{7}$	13 3 $\overline{16}$ 1	10 3 6
6 12 $\overline{18}$ 0	8 2 $\overline{10}$	9 8 $\overline{17}$ 1	9 0 $\overline{8}$	13 4 $\overline{17}$ 0	10 3 7
6 13 $\overline{19}$ 2	9 3 $\overline{10}$	9 9 $\overline{18}$ 0	9 0 $\overline{9}$	13 5 $\overline{18}$ 2	11 2 7
6 14 $\overline{20}$ 1	9 3 $\overline{11}$	9 10 $\overline{19}$ 2	10 1 $\overline{9}$	13 6 $\overline{19}$ 1	11 2 8
		9 11 $\overline{20}$ 1	10 1 $\overline{10}$	13 7 $\overline{20}$ 0	11 2 9
7 0 $\overline{7}$ 1	5 $\overline{2}$ $\overline{2}$				
7 1 $\overline{8}$ 0	5 $\overline{2}$ $\overline{3}$	10 0 $\overline{10}$ 1	7 $\overline{3}$ $\overline{3}$	14 0 $\overline{14}$ 2	10 4 4
7 2 $\overline{9}$ 2	6 $\overline{1}$ $\overline{3}$	10 1 $\overline{11}$ 0	7 $\overline{3}$ $\overline{4}$	14 1 $\overline{15}$ 1	10 4 3
7 3 $\overline{10}$ 1	6 $\overline{1}$ $\overline{4}$	10 2 $\overline{12}$ 2	8 $\overline{2}$ $\overline{4}$	14 2 $\overline{16}$ 0	10 4 6
7 4 $\overline{11}$ 0	6 $\overline{1}$ $\overline{5}$	10 3 $\overline{13}$ 1	8 $\overline{2}$ $\overline{5}$	14 3 $\overline{17}$ 2	11 3 6
7 5 $\overline{12}$ 2	7 0 $\overline{5}$	10 4 $\overline{14}$ 0	8 $\overline{2}$ $\overline{6}$	14 4 $\overline{18}$ 1	11 3 7
7 6 $\overline{13}$ 1	7 0 $\overline{6}$	10 5 $\overline{15}$ 2	9 $\overline{1}$ $\overline{6}$	14 5 $\overline{19}$ 0	11 3 8
7 7 $\overline{14}$ 0	7 0 $\overline{7}$	10 6 $\overline{16}$ 1	9 $\overline{1}$ $\overline{7}$	14 6 $\overline{20}$ 2	12 2 8
7 8 $\overline{15}$ 2	8 1 $\overline{7}$	10 7 $\overline{17}$ 0	9 $\overline{1}$ $\overline{8}$		
7 9 $\overline{16}$ 1	8 1 $\overline{8}$	10 8 $\overline{18}$ 2	10 0 $\overline{8}$	15 0 $\overline{15}$ 0	10 3 3
7 10 $\overline{17}$ 0	8 1 $\overline{9}$	10 9 $\overline{19}$ 1	10 0 $\overline{9}$	15 1 $\overline{16}$ 2	11 4 3
7 11 $\overline{18}$ 2	9 2 $\overline{9}$	10 10 $\overline{20}$ 0	10 0 $\overline{10}$	15 2 $\overline{17}$ 1	11 4 6
7 12 $\overline{19}$ 1	9 2 $\overline{10}$			15 3 $\overline{18}$ 0	11 4 7
7 13 $\overline{20}$ 0	9 2 $\overline{11}$	11 0 $\overline{11}$ 2	8 $\overline{3}$ $\overline{3}$	15 4 $\overline{19}$ 2	12 3 7
		11 1 $\overline{12}$ 1	8 $\overline{3}$ $\overline{4}$	15 5 $\overline{20}$ 1	12 3 8
8 0 $\overline{8}$ 2	6 $\overline{2}$ $\overline{2}$	11 2 $\overline{13}$ 0	8 $\overline{3}$ $\overline{5}$		
8 1 $\overline{9}$ 1	6 $\overline{2}$ $\overline{3}$	11 3 $\overline{14}$ 2	9 $\overline{2}$ $\overline{5}$	16 0 $\overline{16}$ 1	11 3 3
8 2 $\overline{10}$ 0	6 $\overline{2}$ $\overline{4}$	11 4 $\overline{15}$ 1	9 $\overline{2}$ $\overline{6}$	16 1 $\overline{17}$ 0	11 3 6
8 3 $\overline{11}$ 2	7 $\overline{1}$ $\overline{4}$	11 5 $\overline{16}$ 0	9 $\overline{2}$ $\overline{7}$	16 2 $\overline{18}$ 2	12 4 6
8 4 $\overline{12}$ 1	7 $\overline{1}$ $\overline{5}$	11 6 $\overline{17}$ 2	10 $\overline{1}$ $\overline{7}$	16 3 $\overline{19}$ 1	12 4 7
8 5 $\overline{13}$ 0	7 $\overline{1}$ $\overline{6}$	11 7 $\overline{18}$ 1	10 $\overline{1}$ $\overline{8}$	16 4 $\overline{20}$ 0	12 4 8
8 6 $\overline{14}$ 2	8 0 $\overline{6}$	11 8 $\overline{19}$ 0	10 $\overline{1}$ $\overline{9}$		
8 7 $\overline{15}$ 1	8 0 $\overline{7}$	11 9 $\overline{20}$ 2	11 0 $\overline{9}$	17 0 $\overline{17}$ 2	12 3 3
8 8 $\overline{16}$ 0	8 0 $\overline{8}$			17 1 $\overline{18}$ 1	12 3 6
8 9 $\overline{17}$ 2	9 1 $\overline{8}$	12 0 $\overline{12}$ 0	8 4 4	17 2 $\overline{19}$ 0	12 3 7
8 10 $\overline{18}$ 1	9 1 $\overline{9}$	12 1 $\overline{13}$ 2	9 3 4	17 3 $\overline{20}$ 2	13 4 7
8 11 $\overline{19}$ 0	9 1 $\overline{10}$	12 2 $\overline{14}$ 1	9 3 3		
8 12 $\overline{20}$ 2	10 2 $\overline{11}$	12 3 $\overline{15}$ 0	9 3 6	18 0 $\overline{18}$ 0	12 6 6
		12 4 $\overline{16}$ 2	10 2 6	18 1 $\overline{19}$ 2	13 3 6
9 0 $\overline{9}$ 0	6 3 3	12 5 $\overline{17}$ 1	10 2 7	18 2 $\overline{20}$ 1	13 3 7
9 1 $\overline{10}$ 2	7 2 3	12 6 $\overline{18}$ 0	10 2 8		
9 2 $\overline{11}$ 1	7 2 4	12 7 $\overline{19}$ 2	11 $\overline{1}$ 8	19 0 $\overline{19}$ 1	13 6 6
9 3 $\overline{12}$ 0	7 2 3	12 8 $\overline{20}$ 1	11 $\overline{1}$ 9	19 1 $\overline{20}$ 0	13 6 7
				20 0 $\overline{20}$ 2	14 6 6

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Section 4

DIFFRACTION GEOMETRY

4.1-4.6. H. T. EVANS, JR., and K. LONSDALE
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	PAGE
4.1. CLASSIFICATION OF DIFFRACTION METHODS	161
4.2. FIXED-CRYSTAL METHODS	164
4.3. MOVING SINGLE-CRYSTAL METHODS	175
4.4. WEISSENBERG METHOD	185
4.5. BUERGER PRECESSION METHOD	194
4.6. RANDOM-ORIENTATION METHODS	202
4.7. PRECISION MEASUREMENT OF LATTICE PARAMETERS OF POLYCRYSTALLINE SPECIMENS	216

This section classifies the standard methods for resolving, recording and geometrically interpreting diffraction effects from crystals, and presents tables and charts which have proved most useful in connection with these methods.

4.1. Classification of Diffraction Methods

In order to describe any diffraction method completely it is necessary to specify

- (a) the wavelength or range of wavelengths used, together with the geometry of the incident beam.

[A description of the source of radiation (e.g. nature of anticathode, size and uniformity of focus, conditions of running X-ray tube), and details of monochromatization or filtering, collimation (diameter of pinholes, width of slit, amount of divergence or convergence), all help to specify the nature of the incident beam more exactly.]

- (b) The texture of the crystal specimen, its temperature and pressure, orientation and conditions of movement (stationary, oscillating, rotating or precessing)

relative to the incident beam and to the recording device.

- (c) The type and geometry of the recording device (Geiger counter with automatic recording, ionization spectrometer, photographic plane film or plate in front-, side- or back-reflection position, cylindrical camera of stated diameter, etc., position and geometry of screens, pressure and nature of gas in camera) and its position and conditions of movement (if any) relative to both the crystal and crystal movement, and to the incident beam.

The principles and application of various methods and techniques are treated at length in a number of well-known textbooks (General References). They are briefly described here, with reference to the tables applicable to each.

TABLE 4.1.1
Classification of the Main X-ray Diffraction Techniques

Name of technique	Radiation	Condition of specimen	Detecting device
I. Fixed-crystal Methods			
<i>Laue</i>	<i>White (range of λ); collimated</i>	<i>Single crystal; stationary</i>	<i>Photographic</i>
Used for determination of axial ratios and angles; early analysis of simple structures; crystal symmetry (see Vol. I, 3.7); crystal orientation; texture (ideal or mosaic or both in parts, and type of mosaicity) and shape; distinguishing between optical isomers (enantiomorphous, see Vol. I, 4.4), absolute configuration [15, 23]. Geiger-counter techniques are usually unsuitable because the diffracted beams have a wide range of wavelengths (see Section 4.2 and Tables 4.2.1.1A, 4.2.1.1B, 4.2.1.2; general references [8] [9]).			
<i>Stationary crystal</i>	<i>Monochromatic (or filtered characteristic); collimated</i>	<i>Single crystal; stationary</i>	<i>Photographic or Geiger counter</i>
Small unit cell: used for observation of single diffraction effects in order to observe transformation point under, for example, change of temperature or strain [2]. Large unit cell: direct observation of reciprocal lattice, which is of very small mesh [9].			
<i>Diffuse-spot</i>	<i>Monochromatic (or filtered characteristic); collimated</i>	<i>Single crystal; stationary in a succession of positions</i>	<i>Photographic or Geiger counter</i>
Used for observation of "non-Bragg" effects (diffraction outside reciprocal-lattice points), e.g. thermal-vibration waves, incipient crystallization in new phase, disorder, distortion [25] [26]. Interpretation as for 4.3 or individual to each case.			
<i>Kossel or divergent-beam</i>	<i>Monochromatic (usually plus white); divergent</i>	<i>Single crystal; stationary</i>	<i>Photographic; usually plane film</i>

Precision measurements of spacing, texture, symmetry, orientation, Renninger effect [27].

4.1. CLASSIFICATION OF DIFFRACTION METHODS

TABLE 4.1.1 (continued)

Name of technique	Radiation	Condition of specimen	Detecting device
II. Moving Single Crystal and Stationary Film or Detector			
<i>Rotation</i>	<i>Monochromatic (or filtered characteristic); collimated</i>	<i>Single crystal, rotating about zone axis or other principal direction</i>	<i>Photographic or Geiger-counter, or other ionization technique</i>
Repeat distance (identity translation) along rotation axis. Bravais lattice. Axial lengths. Complete analysis of very simple structures (see Section 4.3 and Tables 4.3.2, 4.3.3 [9] [35]).			
<i>Oscillation</i>	<i>Monochromatic (or filtered characteristic); collimated</i>	<i>Single crystal, oscillating through 5°, 10°, 15°, etc., with overlapping settings</i>	<i>Photographic, usually a pack of cylindrical films</i>
Used for crystal setting, for improved resolution as compared with rotation method, for observation of intensities for three-dimensional structure analyses (see Section 4.3, Tables 4.3.2, 4.3.3 [9] [35]).			
<i>Inclined</i>	<i>Monochromatic (or filtered characteristic); collimated</i>	<i>Single crystal, oscillating about axis at known angle to a zone axis</i>	<i>Photographic</i>
Resolution improved, but suitable only for very simple structures. Useful for studying plate-shaped crystals rotated about normal to plane of plate. See [5] [16].			
<i>Random rotation</i>	<i>Monochromatic (or filtered characteristic); collimated</i>	<i>Single crystal, rotating or oscillating about a random direction</i>	<i>Photographic, usually a cylindrical film</i>
Determination of system by multiplicity measurements (Vol. I, 3.5). Identification of rare specimen. Orientation of crystal (especially ground sphere) for purposes of setting [28].			
<i>Multiple exposure</i>	<i>Monochromatic (or filtered characteristic); collimated</i>	<i>Single crystal or powder; under changing conditions</i>	<i>Photographic. Cylindrical film pack, behind screens moved by regular steps</i>
Variation of unit-cell size or intensities with change of conditions. Measurement of phenomena such as "Renninger effect" which depend on crystal orientation. Making of intensity scales [22] [30].			
<i>Geiger-counter diffractometer. Ionization spectrometer</i>	<i>Monochromatic (or filtered characteristic) or characteristic+continuous. Collimated, sometimes by special slit systems</i>	<i>Single crystal, rocked through each reflecting position. (Also powders and fibrous materials, see IV below.)</i>	<i>One- or two-circle Geiger counter, with or without automatic recorder or proportional counter, ionization chamber, scintillation counter</i>
Most accurate determination of positions, integrated intensities and profiles of diffraction spectra. Measurement of wavelengths using standard crystals [9] [31].			
III. Moving Single Crystal and Moving Film or Detector			
<i>Weissenberg</i>	<i>Monochromatic (or filtered characteristic); collimated</i>	<i>Single crystal; rotating or oscillating about zone-axis normal or inclined to incident beam</i>	<i>Cylindrical film (pack) moving behind screens, to and fro parallel to, and synchronously with rotation about the zone axis; sometimes with integrating mechanism or Geiger-counter attachment</i>
Complete data (cell dimensions, lattice type, symmetry, intensities, with or without integrating mechanism) for structure analysis in all systems. Making of intensity scales. Most suitable for crystals where large range of reflections in high-order region is required. See Section 4.4 and Tables 4.4.1–4.4.2 [3] [6] [7] [9]. The Sauter and Schiebold methods are variations of the moving-film technique, less commonly used [3].			

TABLE 4.1.1 (continued)

Name of technique	Radiation	Condition of specimen	Detecting device
III. Moving Single Crystal and Moving Film or Detector (continued)			
<i>Buerger precession</i>	<i>Monochromatic (or filtered characteristic); collimated</i>	<i>Single crystal, oscillating about two mutually-perpendicular zone axes</i>	<i>Plane film (pack) moving behind screens, coupled with crystal so as to be stationary relative to (and parallel to) reciprocal lattice</i>

Most powerful method for determining crystal orientation. Gives data for complete structure analysis, especially for crystals of large unit cells and lower atomic numbers. Gives undistorted image of reciprocal lattice. See Section 4.5, Figs. 4.5.4, 4.5.5, and Tables 4.5.1–4.5.5 [4] [6] [20] [21]. The De-Jong–Bouman method also gives undistorted image of reciprocal lattice, but usually with severely distorted spots (see [3] [19] and Section 4.5, Table 4.5.6).

IV. Random-orientation Methods

<i>Powder (rotating). Debye-Scherrer. Hull</i>	<i>Monochromatic (or filtered characteristic); collimated</i>	<i>Rotating powder or polycrystalline specimen</i>	<i>Photographic or Geiger counter. Focusing camera may be used (Seemann-Bohlin)</i>
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Simple structures (especially metals). Intensity of strong lines (to minimize extinction). Axial ratios of high-symmetry structures. Partial analysis of low-symmetry structures only available as powders. Crystallite size. Transformation conditions. Thermal expansion. Effect on structure of physical changes of other kinds (e.g. ferroelectric, magnetic, antiferromagnetic, pressure, chemical, etc.). Precision data. Comparison of isomorphous crystals. Measurements on series, such as long-chain compounds (variation of lengths of chain, or position of side substituents). Alloys of varying composition. Phase diagrams. Identification of member of series or of mixture. Identification problems in general (finger-print method). See Sections 4.6–4.7 and Tables 4.6, 4.6.2A,B [1] [2] [5] [6] [7] [8] [11] [12]. Principal neutron-diffraction technique [14].

<i>Powder (stationary) (transmission)</i>	<i>Monochromatic (or filtered characteristic); collimated</i>	<i>Powder or other polycrystalline specimen. Stationary</i>	<i>Photographic (usually plane film) or Geiger counter</i>
---	---	---	--

Preferred orientation. Grain size. Strain measurements. Crystallite size in fine powder, dimensions $<10^{-5}$ cm. [1] [2] [6] [7] [8] [11] [12] [13].

<i>Back-reflection method</i>	<i>Monochromatic (or filtered characteristic); collimated</i>	<i>Massive polycrystalline specimen</i>	<i>Plane film surrounding incident beam</i>
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Distortion, grain size, preferred orientation. Correlation with physical properties such as microstructure or hardness [1] [2] [8].

<i>Fibre method</i>	<i>Monochromatic (or filtered characteristic); collimated</i>	<i>Fibrous, stationary or rotating about fibre axis normal to incident beam, or about a normal to the fibre axis</i>	<i>Photographic, usually on plane film, normal to the incident beam</i>
---------------------	---	--	---

Identity period along fibre axis; size, structure and arrangement of micelles; preferred orientation; and determination of orientated textures [6] [8] [9].

<i>Small-angle (low-angle) method</i>	<i>Monochromatic; collimated</i>	<i>Any texture, but in special camera. Non-crystalline material also</i>	<i>Photographic or Geiger counter</i>
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Reference [24].

4.2. Fixed-crystal Methods

For these, as for measurements made on an optical goniometer, standard projection methods, as well as special projection methods, have been extensively used.

4.2.1. Laue Method

All reflections are in general due to different X-ray wavelengths, but all orders of the same spectrum give one single reflection. The symmetry of Laue patterns corresponding to the various point groups is given in Vol. I, Section 3.7.

Laue patterns were originally studied by *stereographic projection of the reflected rays* (W. L. Bragg [31], page 25).

This method has been superseded by the use of
(a) *gnomonic projection* or *of the normals to*
(b) *stereographic projection* *the reflecting planes*

Two cases need to be considered:

1. Plane films, front or back reflections, normal to incident beam.
2. Cylindrical films, cylinder axis normal to incident beam.

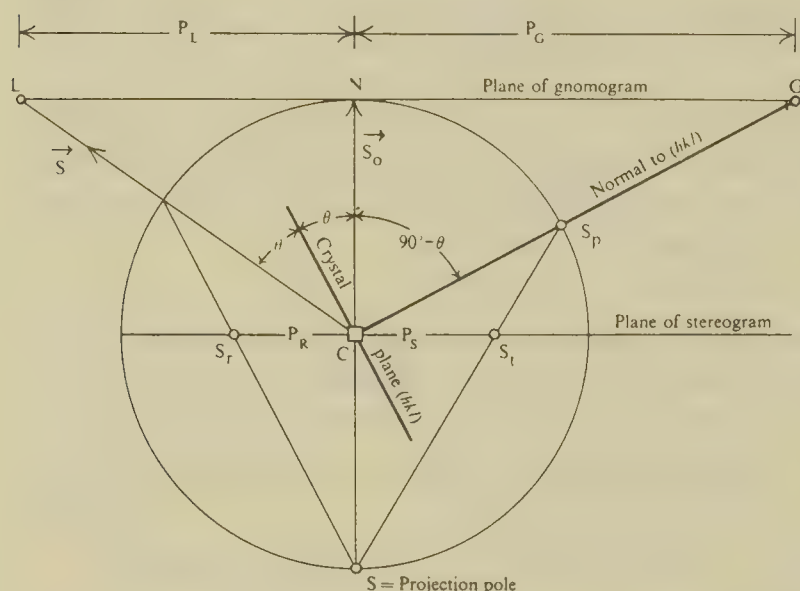


Fig. 4.2.1.1(1) Geometrical principles of the spherical, stereographic, gnomonic and Laue projections.

4.2.1.1. PLANE FILM

Fig. 4.2.1.1(1) shows the graphical relationships involved, for the case of Laue patterns on a plane film, between the incident beam direction SN, which is also the normal to the plane Laue pattern, the Laue pole L and the spherical, stereographic and gnomonic poles, S_p, S_t and G, and the stereographic projection S_r of the reflected beam. If p, the radius of the sphere of projection, is taken equal to r, the crystal-to-film distance, then the planes of gnomonic projection and of the film coincide. The lines producing the various projection poles for any given crystal plane are coplanar with the incident and reflected beams.

In order to transform from one type of projection

to another, the following relationships, given in terms of the Bragg angle θ , are required:

$$P_L = r \tan 2\theta \quad \dots (1)$$

$$P_G = p \cot \theta \quad \dots (2)$$

$$P_S = p \frac{\cos \theta}{1 + \sin \theta} \quad \dots (3)$$

For the stereographic projection of the *reflected ray* on to the equatorial plane

$$P_R = p \tan \theta \quad \dots (4)$$

Tables 4.2.1.1A and B give corresponding values of P_L , P_S , P_G for the front- and back-reflection regions respectively over a range of angles of deviation of 2θ .

$$\begin{aligned} \text{For Table 4.2.1.1A: } r=5 \text{ cm } & \begin{cases} p=15 \text{ cm for } P_S \\ p=2 \text{ cm for } P_G \end{cases} \\ \text{For Table 4.2.1.1B: } r=5 \text{ cm } & \begin{cases} p=15 \text{ cm for } P_S \\ p=50 \text{ cm for } P_G \end{cases} \end{aligned}$$

These values of p are chosen because they give convenient ranges of P_S and of P_G , but if other values of r or p are used, appropriate adjustments must be made.

These tables are not intended for direct use. They may be plotted as graphs; or straight stereographic or gnomonic rulers may be constructed for suitable values of r and p. Such a ruler has P_L to the left, $P_S(P_G)$ to the right of a pivot which is placed at the centre of the photograph (origin of the projection). Corresponding poles L, S_t(G) are numbered to correspond to each other, and it is therefore simple to transform the Laue pattern directly to the stereographic or gnomonic projection without intermediate measurements. If either projection is subsequently to be used with a stereographic or gnomonic net, the scale must be adjusted. For a stereographic net of diameter 2x cm the P_S numbers in Tables 4.2.1.1A and B must be multiplied by x/15.

The use of a stereographic net is described in many textbooks, and in general the charts commercially available (Sec. 1.2, p. 1) are excellent, being much more accurate than most people can draw them. They are, however, of particular sizes and are therefore not suitable for every use without accurate enlargement.

A description of the stereographic, gnomonic and other nets and types of projection and a comparison of their advantages and disadvantages are given by Henry, Lipson and Wooster [9].

Various nets may be constructed as follows:

Polar Stereographic Net

- (a) Concentric circles of radii $p \tan \phi/2$, where p is the radius of the projection circle and ϕ the angle between the directions (CN, CS_p in Fig. 4.2.1.1(1)) of the projection diameter and the projected radius. ϕ is usually varied by 2° from 0° to 90°.
- (b) Intersecting these circles are a set of regularly-spaced diameters at, say, 2° intervals.

4.2. FIXED-CRYSTAL METHODS

TABLE 4.2.1.1A

Table for Conversion of Front-reflection Laue Patterns to Stereographic or Gnomonic Projections

See page 164 for explanation of this table

2θ	$P_{L(t)}$ r=5 cm	P_S p=15 cm	P_G p=2 cm	2θ	$P_{L(t)}$ r=5 cm	P_S p=15 cm	P_G p=2 cm
0°	0	15	∞	30°	2.887	11.51	7.464
1	0.0873	14.87	229.2	31	3.004	11.41	7.212
2	0.1746	14.74	114.6	32	3.124	11.30	6.975
3	0.262	14.61	76.38	33	3.247	11.20	6.752
4	0.350	14.48	57.27	34	3.373	11.10	6.542
5°	0.437	14.36	45.81	35°	3.501	11.00	6.343
6	0.526	14.23	38.16	36	3.633	10.90	6.155
7	0.614	14.11	32.70	37	3.768	10.80	5.977
8	0.703	13.99	28.60	38	3.906	10.70	5.808
9	0.792	13.87	25.41	39	4.049	10.60	5.648
10°	0.882	13.74	22.86	40°	4.195	10.50	5.495
11	0.972	13.62	20.77	41	4.346	10.41	5.349
12	1.063	13.51	19.029	42	4.502	10.31	5.210
13	1.154	13.39	17.554	43	4.663	10.21	5.077
14	1.247	13.27	16.289	44	4.828	10.12	4.950
15°	1.340	13.15	15.192	45°	5.000	10.02	4.828
16	1.434	13.04	14.231	46	5.178	9.93	4.712
17	1.529	12.93	13.382	47	5.362	9.83	4.600
18	1.625	12.81	12.628	48	5.553	9.74	4.492
19	1.722	12.70	11.952	49	5.752	9.65	4.389
20°	1.820	12.59	11.343	50°	5.959	9.56	4.289
21	1.919	12.48	10.791	51	6.174	9.46	4.193
22	2.020	12.37	10.289	52	6.400	9.37	4.101
23	2.122	12.26	9.830	53	6.635	9.28	4.011
24	2.226	12.15	9.409	54	6.882	9.19	3.925
25°	2.332	12.04	9.021	55°	7.141	9.10	3.842
26	2.439	11.93	8.663	56	7.413	9.01	3.761
27	2.548	11.83	8.331	57	7.699	8.92	3.684
28	2.659	11.72	8.022	58	8.002	8.84	3.608
29	2.772	11.61	7.733	59	8.321	8.75	3.535

4.2. FIXED-CRYSTAL METHODS

TABLE 4.2.1.1B

Table for Conversion of Back-reflection Laue Patterns to Stereographic or Gnomonic Projections

See page 164 for explanation of this table

2θ	$P_{L(b)}$ $r=5\text{ cm}$	P_S $p=15\text{ cm}$	P_G $p=50\text{ cm}$	2θ	$P_{L(b)}$ $r=5\text{ cm}$	P_S $p=15\text{ cm}$	P_G $p=50\text{ cm}$
120°	8.660	4.019	28.868	150°	2.887	1.975	13.398
121	8.321	3.949	28.289	151	2.772	1.908	12.931
122	8.002	3.877	27.716	152	2.659	1.842	12.467
123	7.699	3.809	27.148	153	2.548	1.775	12.004
124	7.413	3.740	26.586	154	2.439	1.709	11.544
125°	7.141	3.671	26.029	155°	2.332	1.643	11.085
126	6.882	3.601	25.477	156	2.226	1.577	10.628
127	6.635	3.532	24.929	157	2.122	1.510	10.173
128	6.400	3.463	24.387	158	2.020	1.444	9.719
129	6.174	3.394	23.849	159	1.919	1.378	9.267
130°	5.959	3.326	23.316	160°	1.820	1.312	8.817
131	5.752	3.257	22.787	161	1.722	1.246	8.367
132	5.553	3.188	22.262	162	1.625	1.181	7.919
133	5.362	3.120	21.741	163	1.529	1.115	7.473
134	5.178	3.052	21.224	164	1.434	1.049	7.027
135°	5.000	2.984	20.711	165°	1.340	0.983	6.583
136	4.828	2.916	20.202	166	1.247	0.917	6.139
137	4.663	2.848	19.696	167	1.154	0.852	5.697
138	4.502	2.780	19.193	168	1.063	0.786	5.255
139	4.346	2.713	18.694	169	0.972	0.720	4.815
140°	4.195	2.645	18.199	170°	0.882	0.655	4.375
141	4.049	2.578	17.706	171	0.792	0.589	3.935
142	3.906	2.510	17.217	172	0.703	0.524	3.497
143	3.768	2.443	16.730	173	0.614	0.458	3.058
144	3.633	2.376	16.246	174	0.526	0.393	2.621
145°	3.501	2.309	15.765	175°	0.437	0.327	2.183
146	3.373	2.242	15.287	176	0.350	0.262	1.746
147	3.247	2.175	14.811	177	0.262	0.196	1.310
148	3.124	2.108	14.338	178	0.175	0.131	0.873
149	3.004	2.041	13.866	179	0.087	0.065	0.437

Wulff Stereographic Net

Two sets of circles or arcs of circles, each set having collinear centres, the lines of centres being normal to each other, through the centre O of the projection circle, radius p.

(a) Centres at $\pm p \operatorname{cosec} \phi$ from O, radius $p \cot \phi$.

(b) Centres at $\pm p \cot \phi$ from O, radius $p \operatorname{cosec} \phi$.

Gnomonic Net

(a) Parallel straight lines at intervals $\pm p \tan \phi$ from an equatorial line (through N and normal to the plane of the paper in Fig. 4.2.1.1(1)), intersected by

(b) Symmetrical coplanar hyperbolae of equations

$$y^2 = p^2(1+x^2) \tan^2 \phi$$

where $y=0$ is normal to set (a) and $x=0$ is the equatorial line of set (a).

A detailed discussion of the construction of stereographic and gnomonic nets, suitable for self-teaching, is to be found in W. P. Davey's *Study of Crystal Structure and its Applications* (McGraw-Hill, New York and London, 1934), which, however, is now out of print. See also H. Tertsch [34].

Greninger Chart

This is used for reading angular relations on back-reflection Laue photographs. It provides a quick way of determining the orientation of a single crystal, or the relative orientations of two individual grains in an aggregate or of the components of a twin.

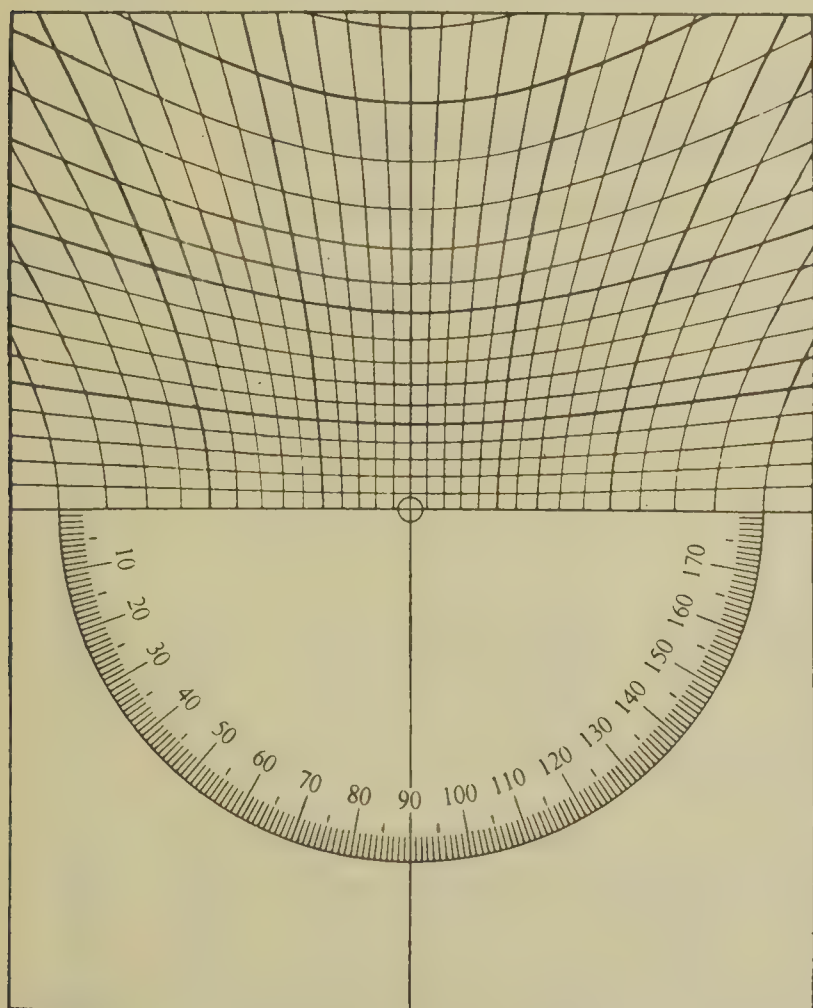


Fig. 4.2.1.1(2). Greninger chart [32].

It has to be constructed for a particular crystal-to-film distance, and it consists essentially of two sets of curves, the formulae of which are given by Bernalte, A. (1965), *Acta Cryst.*, **19**, 916, together with a half-circle protractor (Fig. 4.2.1.1(2)) [32].

An excellent description of the use of this chart is given by C. S. Barrett [2], pages 167–72.

4.2.1.2. CYLINDRICAL FILM

A special chart is used for the interpretation of a Laue pattern on a cylindrical film, cylinder axis normal to the incident beam. The data for the construction of such a chart, given in Tables 4.2.1.2A, B, C, D, are obtained as follows.

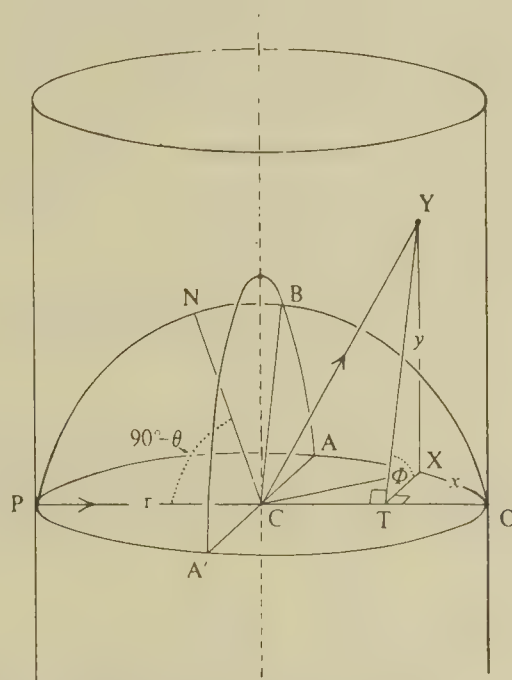


Fig. 4.2.1.2(1). Geometrical principles of Laue photography on to a cylindrical film with axis normal to the incident beam.

In Fig. 4.2.1.2(1), PO is the incident beam (S_0), CN the normal to the reflecting plane, and CY the diffracted beam (S), Y being the point in which CY intersects the cylindrical film, giving a Laue spot.

PXO is the equatorial plane, normal to the cylinder axis. Let YX be normal to PXO; XT and YT normal to CO. Then $\angle OCY = 2\theta$, where θ is the Bragg angle. YT is coplanar with PO, CN and CY, and therefore $\angle XTY = \phi$ is the angle between the equatorial plane and the plane of incidence. The direction CN is fully specified by θ and ϕ , and if these are known, the positions of the normals to the reflecting planes can be plotted on a stereographic net.

When the film is laid flat, the position of each spot Y is specified by Cartesian co-ordinates x (arc OX) and $y = YX$. Let the cylinder radius be r. Note that $\angle YCX = \chi$, $\angle XCT = \psi$ in Buerger's notation (see Table 4.3.1, page 175).

4.2. FIXED-CRYSTAL METHODS

$$\cos 2\theta = \cos \chi \cdot \cos \Upsilon = \cos \left(\tan^{-1} \frac{y}{r} \right) \cos \frac{x}{r} \dots (1)$$

$$\text{Also } y = XT \tan \Phi = r \sin \frac{x}{r} \tan \Phi \dots (2)$$

For a cylindrical camera of radius 28.65 mm and if x and y are measured in mm. these equations reduce to

$$\cos 2\theta = \cos \left(\tan^{-1} \frac{y}{28.65} \right) \cos 2x \dots (3)$$

$$y = 28.65 \sin 2x \cdot \tan \Phi \dots (4)$$

the angles being expressed in degrees.

In Table 4.2.1.2A, y is given in terms of x and Φ for $\Phi = 1^\circ$ to $\Phi = 70^\circ$. For lines with $\Phi = 51^\circ$ to $\Phi = 90^\circ$ the separation of points to be plotted which have low x values (5, 10, 15, 20 mm) is large, and this separation increases rapidly as Φ increases. To overcome difficulties in plotting lines in this region, Table 4.2.1.2B gives x in terms of y and Φ , for $\Phi = 51^\circ$ to $\Phi = 90^\circ$.

For Φ less than 71° , Table 4.2.1.2B by itself gives widely separated points in the region $x = 35$ mm to $x = 45$ mm. The range $y = 0$ to $y = 80$ mm covers the size of films normally used.

Table 4.2.1.2C gives x in terms of y and θ , for $\theta = 0^\circ$ to $\theta = 45^\circ$. Extra points to facilitate drawing are given in Table 4.2.1.2D, where y is tabulated for $x = 0$ and $x = 5$ mm for $\theta = 0^\circ$ to $\theta = 45^\circ$.

The chart obtained from these tables consists of two families of curves (a) of constant θ and (b) of constant Φ . The figures given in the tables cover the one-eighth

of the film limited by $y = 0$, $y = 80$ mm, $x = 0$ and $x = 45$ mm. Reference to Fig. 4.2.1.2(3) shows how the rest of the chart for Φ up to 360° and θ to 90° is obtained by symmetry operations on this unit. The accuracy of the tabulated figures varies from place to place on the chart but should be within 0.02 mm.

If a camera of any other radius is used, either x and y can be corrected to correspond to a camera of radius 28.65 mm, or equations (1) and (2) can be used to give new figures, or the chart can be enlarged to the required size.

The angles θ and Φ , read off from the chart laid over the film, can be used to plot a stereogram as follows:

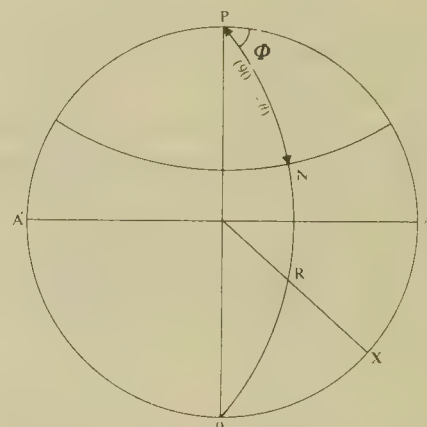


Fig. 4.2.1.2(2). Stereographic projection showing the direction of the reflected beam R from planes having the normal N defined by the angles $(90^\circ - \theta)$ and Φ . R is the direction CY in Fig. 4.2.1.2(1).

TABLE 4.2.1.2

Tables for Conversion of Cylindrical Laue Patterns to Stereographic Projections

Prepared by M. CANUT and checked by I. E. KNAGGS and G. BULLEN

For layout see Fig. 4.2.1.2(3). The tabulated figures give a convenient scale for drafting, but the chart may be reduced photographically to any required diameter size of camera, for direct use with film.

TABLE 4.2.1.2A. Table of y in terms of x and Φ . (x and y in mm and Φ in degrees. $r = 28.65$ mm.)

Φ x	1	2	3	4	5	6	7	8	9	10	11	12
0	0	0	0	0	0	0	0	0	0	0	0	0
5	0.09	0.17	0.26	0.35	0.44	0.52	0.61	0.70	0.79	0.88	0.97	1.06
10	0.17	0.34	0.51	0.69	0.86	1.03	1.20	1.38	1.55	1.73	1.91	2.08
15	0.25	0.50	0.75	1.00	1.25	1.51	1.76	2.01	2.27	2.53	2.79	3.05
20	0.32	0.64	0.97	1.29	1.61	1.94	2.26	2.59	2.92	3.25	3.58	3.92
25	0.38	0.77	1.15	1.54	1.92	2.31	2.70	3.09	3.48	3.87	4.27	4.67
30	0.43	0.87	1.30	1.74	2.17	2.61	3.05	3.49	3.93	4.38	4.82	5.27
35	0.47	0.94	1.41	1.88	2.36	2.83	3.31	3.78	4.27	4.75	5.23	5.72
40	0.49	0.99	1.48	1.97	2.47	2.97	3.46	3.97	4.47	4.98	5.49	6.00
45	0.50	1.00	1.50	2.00	2.51	3.01	3.52	4.03	4.54	5.05	5.57	6.09

4.2. FIXED-CRYSTAL METHODS

TABLE 4.2.1.2A (continued)

Φ x	13	14	15	16	17	18	19	20	21	22	23	24
0	0	0	0	0	0	0	0	0	0	0	0	0
5	1.15	1.24	1.33	1.43	1.52	1.62	1.71	1.81	1.91	2.01	2.11	2.21
10	2.26	2.44	2.63	2.81	3.00	3.18	3.38	3.57	3.76	3.96	4.16	4.36
15	3.31	3.57	3.84	4.11	4.38	4.66	4.93	5.22	5.50	5.79	6.08	6.38
20	4.25	4.59	4.94	5.28	5.63	5.99	6.34	6.71	7.07	7.44	7.82	8.20
25	5.07	5.47	5.88	6.30	6.71	7.13	7.56	7.99	8.43	8.87	9.32	9.77
30	5.73	6.19	6.65	7.12	7.59	8.06	8.55	9.03	9.53	10.02	10.53	11.05
35	6.22	6.71	7.22	7.72	8.23	8.75	9.27	9.80	10.34	10.88	11.43	11.99
40	6.52	7.04	7.56	8.09	8.63	9.17	9.72	10.27	10.83	11.40	11.98	12.57
45	6.62	7.15	7.68	8.22	8.76	9.31	9.87	10.43	11.00	11.58	12.16	12.76

Φ x	25	26	27	28	29	30	31	32	33	34	35	36
0	0	0	0	0	0	0	0	0	0	0	0	0
5	2.32	2.43	2.54	2.65	2.76	2.87	2.99	3.11	3.23	3.36	3.48	3.61
10	4.57	4.78	4.99	5.21	5.43	5.66	5.89	6.13	6.37	6.61	6.86	7.12
15	6.68	6.99	7.30	7.62	7.94	8.27	8.61	8.95	9.31	9.67	10.03	10.41
20	8.59	8.99	9.39	9.80	10.21	10.63	11.07	11.51	11.96	12.43	12.90	13.39
25	10.23	10.71	11.18	11.67	12.17	12.68	13.19	13.72	14.26	14.81	15.37	15.95
30	11.57	12.11	12.65	13.19	13.76	14.32	14.91	15.51	16.12	16.74	17.38	18.03
35	12.56	13.13	13.72	14.32	14.93	15.54	16.18	16.83	17.49	18.17	18.86	19.57
40	13.16	13.76	14.38	15.01	15.65	16.29	16.96	17.64	18.33	19.03	19.76	20.51
45	13.37	13.98	14.60	15.24	15.89	16.54	17.22	17.91	18.61	19.33	20.06	20.82

Φ x	37	38	39	40	41	42	43	44	45	46	47	48
0	0	0	0	0	0	0	0	0	0	0	0	0
5	3.75	3.89	4.03	4.18	4.33	4.48	4.64	4.80	4.97	5.15	5.33	5.52
10	7.39	7.66	7.94	8.22	8.52	8.83	9.14	9.47	9.80	10.15	10.51	10.89
15	10.80	11.19	11.60	12.02	12.46	12.90	13.37	13.84	14.33	14.84	15.37	15.91
20	13.88	14.39	14.92	15.45	16.02	16.59	17.18	17.78	18.42	19.08	19.75	20.46
25	16.54	17.15	17.78	18.42	19.09	19.77	20.47	21.20	21.96	22.74	23.54	24.37
30	18.70	19.39	20.10	20.82	21.58	22.35	23.14	23.96	24.81	25.69	26.61	27.56
35	20.29	21.04	21.81	22.59	23.41	24.25	25.11	26.00	26.93	27.89	28.88	29.91
40	21.27	22.05	22.86	23.68	24.53	25.41	26.32	27.25	28.22	29.23	30.26	31.35
45	21.60	22.39	23.21	24.04	24.91	25.80	26.72	27.67	28.65	29.68	30.73	31.83

4.2. FIXED-CRYSTAL METHODS

TABLE 4.2.1.2A (continued)

Φ x	49	50	51	52	53	54	55	56	57	58	59	60
0	0	0	0	0	0	0	0	0	0	0	0	0
5	5.72	5.93	6.15	6.37	6.60	6.85	7.11	7.38	7.66	7.96	8.28	8.62
10	11.27	11.68	12.11	12.55	13.01	13.49	14.00	14.53	15.09	15.69	16.31	16.98
15	16.48	17.08	17.69	18.34	19.01	19.72	20.46	21.24	22.07	22.93	23.84	24.81
20	21.19	21.96	22.75	23.58	24.44	25.35	26.31	27.31	28.37	29.48	30.66	31.91
25	25.25	26.16	27.11	28.10	29.13	30.21	31.34	32.54	33.80	35.12	36.52	38.01
30	28.55	29.57	30.64	31.76	32.93	34.15	35.44	36.79	38.21	39.71	41.29	42.98
35	30.97	32.09	33.25	34.46	35.74	37.06	38.46	39.92	41.47	43.09	44.81	46.64
40	32.46	33.63	34.85	36.12	37.46	38.84	40.31	41.84	43.46	45.17	46.97	48.89
45	32.96	34.15	35.38	36.68	38.03	39.44	40.93	42.48	44.13	45.85	47.68	49.62

Φ x	61	62	63	64	65	66	67	68	69	70
0	0	0	0	0	0	0	0	0	0	0
5	8.98	9.36	9.77	10.20	10.67	11.18	11.72	12.32	12.96	13.67
10	17.68	18.43	19.24	20.10	21.02	22.02	23.09	24.26	25.54	26.93
15	25.84	26.94	28.11	29.38	30.73	32.18	33.75	35.46	37.33	39.37
20	33.23	34.64	36.15	37.77	39.50	41.37	43.39	45.59	47.98	50.60
25	39.59	41.27	43.07	45.00	47.06	49.29	51.70	54.32	57.17	60.30
30	44.76	46.67	48.70	50.88	53.21	55.73	58.45	61.42	64.64	68.17
35	48.57	50.64	52.84	55.21	57.75	60.47	63.43	66.65	70.15	73.98
40	50.91	53.08	55.39	57.86	60.52	63.39	66.48	69.85	73.52	77.54
45	51.69	53.89	56.23	58.75	61.45	64.36	67.50	70.93	74.64	78.72

TABLE 4.2.1.2B. Φ -lines. Table of x in terms of y and Φ . (x and y in mm and Φ in degrees. $r=28.65$ mm.)

Φ y	51	52	53	54	55	56	57	58	59	60	61	62	63
0	0	0	0	0	0	0	0	0	0	0	0	0	0
5	4.06	3.92	3.78	3.64	3.51	3.38	3.26	3.13	3.01	2.89	2.78	2.66	2.55
10	8.21	7.92	7.63	7.35	7.08	6.81	6.55	6.30	6.06	5.82	5.58	5.35	5.13
15	12.55	12.08	11.62	11.19	10.76	10.34	9.94	9.56	9.17	8.80	8.44	8.09	7.74
20	17.22	16.53	15.87	15.24	14.64	14.05	13.48	12.94	12.41	11.89	11.39	10.90	10.42
25	22.49	21.50	20.56	19.68	18.84	18.04	17.27	16.53	15.82	15.13	14.47	13.83	13.21
30	29.00	27.45	26.05	24.77	23.57	22.47	21.42	20.44	19.50	18.60	17.74	16.92	16.13
35	40.80	36.33	33.52	31.29	29.41	27.75	26.25	24.89	23.62	22.43	21.32	20.26	19.26
40					38.94	35.19	32.53	30.38	28.52	26.86	25.36	23.98	22.69
45								39.48	35.35	32.55	30.26	28.33	26.59
50											37.67	34.06	31.39
55													39.00

4.2. FIXED-CRYSTAL METHODS

TABLE 4.2.1.2B (continued)

Φ y	64	65	66	67	68	69	70	71	72	73	74	75	76
0	0	0	0	0	0	0	0	0	0	0	0	0	0
5	2.44	2.34	2.23	2.13	2.02	1.92	1.82	1.73	1.63	1.53	1.44	1.34	1.25
10	4.90	4.69	4.47	4.26	4.06	3.85	3.65	3.45	3.26	3.07	2.87	2.69	2.50
15	7.40	7.07	6.74	6.43	6.11	5.80	5.50	5.20	4.90	4.61	4.32	4.04	3.75
20	9.96	9.50	9.06	8.62	8.19	7.78	7.36	6.96	6.56	6.17	5.78	5.39	5.02
25	12.60	12.01	11.44	10.88	10.33	9.79	9.26	8.75	8.24	7.74	7.25	6.77	6.29
30	15.36	14.62	13.90	13.20	12.52	11.85	11.21	10.57	9.95	9.34	8.74	8.15	7.57
35	18.29	17.37	16.48	15.62	14.79	13.99	13.21	12.44	11.70	10.97	10.26	9.56	8.87
40	21.47	20.32	19.22	18.18	17.17	16.21	15.28	14.37	13.49	12.64	11.81	10.99	10.19
45	25.01	23.56	22.19	20.92	19.70	18.55	17.44	16.38	15.35	14.36	13.39	12.45	11.53
50	29.17	27.24	25.49	23.90	22.42	21.03	19.72	18.47	17.27	16.12	15.02	13.94	12.90
55	34.71	31.77	29.36	27.30	25.44	23.74	22.17	20.69	19.29	17.97	16.71	15.49	14.30
60		38.79	34.41	31.38	28.89	26.75	24.84	23.08	21.44	19.90	18.45	17.07	15.74
65				37.20	33.22	30.29	27.84	25.69	23.75	21.96	20.29	18.72	17.23
70					40.41	34.86	31.40	28.64	26.28	24.17	22.24	20.45	18.77
75							36.17	32.17	29.14	26.58	24.32	22.28	20.37
80								37.02	32.57	29.31	26.61	24.22	22.07

Φ y	77	78	79	80	81	82	83	84	85	86	87	88	89	90
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5	1.16	1.07	0.97	0.88	0.79	0.70	0.62	0.53	0.44	0.35	0.26	0.18	0.09	0
10	2.31	2.13	1.95	1.77	1.59	1.41	1.23	1.05	0.88	0.70	0.53	0.35	0.18	0
15	3.48	3.20	2.92	2.65	2.38	2.11	1.84	1.58	1.32	1.05	0.79	0.53	0.26	0
20	4.64	4.27	3.90	3.54	3.18	2.82	2.46	2.11	1.75	1.40	1.05	0.70	0.35	0
25	5.82	5.35	4.89	4.43	3.98	3.53	3.08	2.64	2.19	1.75	1.31	0.88	0.44	0
30	7.00	6.43	5.87	5.32	4.78	4.24	3.69	3.16	2.63	2.10	1.58	1.05	0.53	0
35	8.19	7.53	6.87	6.22	5.58	4.94	4.32	3.69	3.07	2.45	1.84	1.23	0.61	0
40	9.41	8.64	7.88	7.13	6.39	5.66	4.94	4.22	3.51	2.80	2.10	1.40	0.70	0
45	10.64	9.76	8.89	8.04	7.21	6.38	5.56	4.75	3.95	3.16	2.36	1.58	0.79	0
50	11.88	10.89	9.92	8.96	8.02	7.10	6.19	5.29	4.39	3.51	2.63	1.75	0.88	0
55	13.16	12.05	10.96	9.89	8.85	7.83	6.82	5.82	4.84	3.86	2.89	1.93	0.96	0
60	14.46	13.22	12.01	10.84	9.69	8.56	7.45	6.36	5.28	4.21	3.15	2.10	1.05	0
65	15.80	14.42	13.09	11.79	10.53	9.30	8.09	6.90	5.73	4.57	3.42	2.28	1.14	0
70	17.17	15.65	14.18	12.76	11.39	10.04	8.73	7.44	6.17	4.92	3.68	2.45	1.22	0
75	18.59	16.91	15.30	13.74	12.25	10.79	9.38	7.99	6.62	5.28	3.94	2.63	1.31	0
80	20.07	18.22	16.45	14.76	13.13	11.56	10.03	8.54	7.08	5.64	4.21	2.80	1.40	0

4.2. FIXED-CRYSTAL METHODS

TABLE 4.2.1.2C. θ -lines. Table of x in terms of y and θ . (x and y in mm and θ in degrees. $r=28.65$ mm.)

$\theta \backslash y$	0	1	2	3	4	5	6	7	8	9	10	11
0	0	1.00	2.00	3.00	4.00	5.00	6.00	7.00	8.00	9.00	10.00	11.00
$2\frac{1}{2}$				$\simeq 1.65$	3.14	4.34	5.48	6.57				
5						$\simeq 0.7$	3.42	4.99	6.32	7.56	8.74	9.87
$7\frac{1}{2}$									$\simeq 3.25$	5.27	6.87	8.28
10											$\simeq 2.75$	5.43

$\theta \backslash y$	12	13	14	15	16	17	18	19	20	21	22	23
0	12.00	13.00	14.00	15.00	16.00	17.00	18.00	19.00	20.00	21.00	22.00	23.00
5	11.00	12.08	13.17	14.24	15.30	16.35	17.39	18.44	19.48	20.52	21.55	22.58
10	7.31	8.90	10.37	11.74	13.04	14.29	15.51	16.71	17.88	19.04	20.19	21.31
$12\frac{1}{2}$	$\simeq 2.33$	5.64	7.79	9.56								
15			$\simeq 2.36$	6.10	8.42	10.32	12.02	13.60	15.07	16.49	17.86	19.18
$17\frac{1}{2}$					$\simeq 3.24$	6.87	9.28					
20							$\simeq 4.67$	8.04	10.44	12.50	14.35	16.04
25										$\simeq 4.71$	8.66	11.39

$\theta \backslash y$	24	25	26	27	28	29	30	31	32	33	34	35
0	24.00	25.00	26.00	27.00	28.00	29.00	30.00	31.00	32.00	33.00	34.00	35.00
5	23.61	24.64	25.67	26.69	27.71	28.73	29.75	30.77	31.79	32.81	33.83	34.84
10	22.44	23.54	24.65	25.75	26.84	27.93	29.01	30.09	31.17	32.24	33.31	34.38
15	20.48	21.74	22.99	24.22	25.43	26.64	27.82	29.00	30.18	31.34	32.49	33.65
20	17.66	19.19	20.68	22.11	23.50	24.86	26.22	27.54	28.84	30.14	31.41	32.67
25	13.68	15.72	17.60	19.36	21.04	22.65	24.21	25.73	27.21	28.67	30.09	31.50
30	7.16	10.72	13.47	15.84	17.96	19.94	21.80	23.59	25.30	26.96	28.58	30.16
35			6.82	10.95	14.01	16.61	18.94	21.09	23.11	25.03	26.87	28.66
40					8.08	12.24	15.41	18.14	20.59	22.84	24.98	27.01
45						4.67	10.70	14.53	17.65	20.39	22.89	25.22
50								9.57	14.05	17.54	20.55	23.26
55									9.20	14.16	17.91	21.11
60										9.64	14.80	18.73
65											10.88	16.00
70											4.24	12.71
75												8.28

4.2. FIXED-CRYSTAL METHODS

TABLE 4.2.1.2C (continued)

θ y	36	37	38	39	40	41	42	43	44	45
0	36.00	37.00	38.00	39.00	40.00	41.00	42.00	43.00	44.00	45.00
5	35.86	36.88	37.89	38.91	39.93	40.94	41.96	42.97	43.99	45.00
10	35.45	36.52	37.58	38.64	39.70	40.76	41.82	42.89	43.94	45.00
15	34.79	35.94	37.08	38.22	39.35	40.48	41.61	42.74	43.87	45.00
20	33.93	35.18	36.42	37.66	38.89	40.12	41.34	42.56	43.78	45.00
25	32.89	34.27	35.64	36.99	38.34	39.68	41.02	42.34	43.68	45.00
30	31.71	33.24	34.75	36.24	37.72	39.19	40.65	42.10	43.55	45.00
35	30.40	32.11	33.77	35.42	37.04	38.66	40.25	41.84	43.42	45.00
40	28.97	30.88	32.73	34.54	36.33	38.09	39.83	41.56	43.29	45.00
45	27.44	29.57	31.62	33.62	35.57	37.49	39.39	41.27	43.14	45.00
50	25.78	28.17	30.44	32.64	34.78	36.87	38.94	40.97	42.99	45.00
55	24.00	26.69	29.21	31.62	33.96	36.23	38.46	40.66	42.84	45.00
60	22.09	25.12	27.92	30.57	33.12	35.58	37.98	40.34	42.68	45.00
65	19.99	23.44	26.57	29.49	32.25	34.91	37.49	40.02	42.52	45.00
70	17.66	21.65	25.15	28.35	31.36	34.22	36.99	39.69	42.36	45.00
75	15.00	19.71	23.65	27.18	30.44	33.52	36.49	39.37	42.19	45.00
80	11.78	17.58	22.07	25.96	29.50	32.81	35.97	39.03	42.03	45.00

TABLE 4.2.1.2D. θ -lines. Table of y in terms of x and θ . (x and y in mm and θ in degrees. $r=28.65$ mm.)

θ x	0	1	2	3	4	5	6	7	8	9	10	11
0	0	1.00	2.00	3.01	4.03	5.05	6.09	7.15	8.22	9.31	10.43	11.58
5						0	3.38	5.00	6.39	7.71	9.00	10.27

θ x	12	13	14	15	16	17	18	19	20	21	22	23
0	12.76	13.98	15.24	16.54	17.91	19.33	20.82	22.39	24.04	25.80	27.67	29.68
5	11.55	12.83	14.17	15.52	16.92	18.38	19.90	21.49	23.15	24.93	26.80	28.80

θ x	24	25	26	27	28	29	30	31	32	33	34	35
0	31.83	34.15	36.68	39.44	42.48	45.85	49.64	53.89	58.75	64.36	70.93	78.72
5	30.95	33.26	35.77	38.52	41.53	44.89	48.64	52.84	57.64	63.18	69.66	77.36

4.2. FIXED-CRYSTAL METHODS

ABA' in Fig. 4.2.1.2(1) is a circle centre C, radius r , normal to PC. Let A, A' and B be the points of intersection of this circle with the circles PXO and PNO respectively (equatorial plane and plane of incidence).

$$\angle PCN = 90^\circ - \theta$$

Hence $\angle NCB = \theta$ and $\angle BCA = \angle YTX = \Phi$

If the cylinder axis is taken as the projection diameter and PAO as the plane of the stereogram, then E is the stereographic projection of N (Fig. 4.2.1.2(2)).

NOTE. The chart shown in Fig. 4.2.1.2(3) is similar to that given by C. S. Barrett [2], page 164, but he uses α instead of Φ . As reproduced for sale, ρ is sometimes used instead of $90^\circ - \theta$, ϕ instead of Φ . A similar chart

is also given on page 638 of Vol. II, Internationale Tabellen zur Bestimmung von Krystallstrukturen, to which reference is made for various other configurations of crystal, beam and film [33].

4.2.2. Divergent-beam Method

No tables are presented for this method, which is not in wide use.

The pattern is obtained on a plane or cylindrical film and may be compared with a calculated pattern. For this purpose gnomonic, orthogonal (Kossel), cylindrical or stereographic-projection methods may be used. Reference should be made to original papers [27].

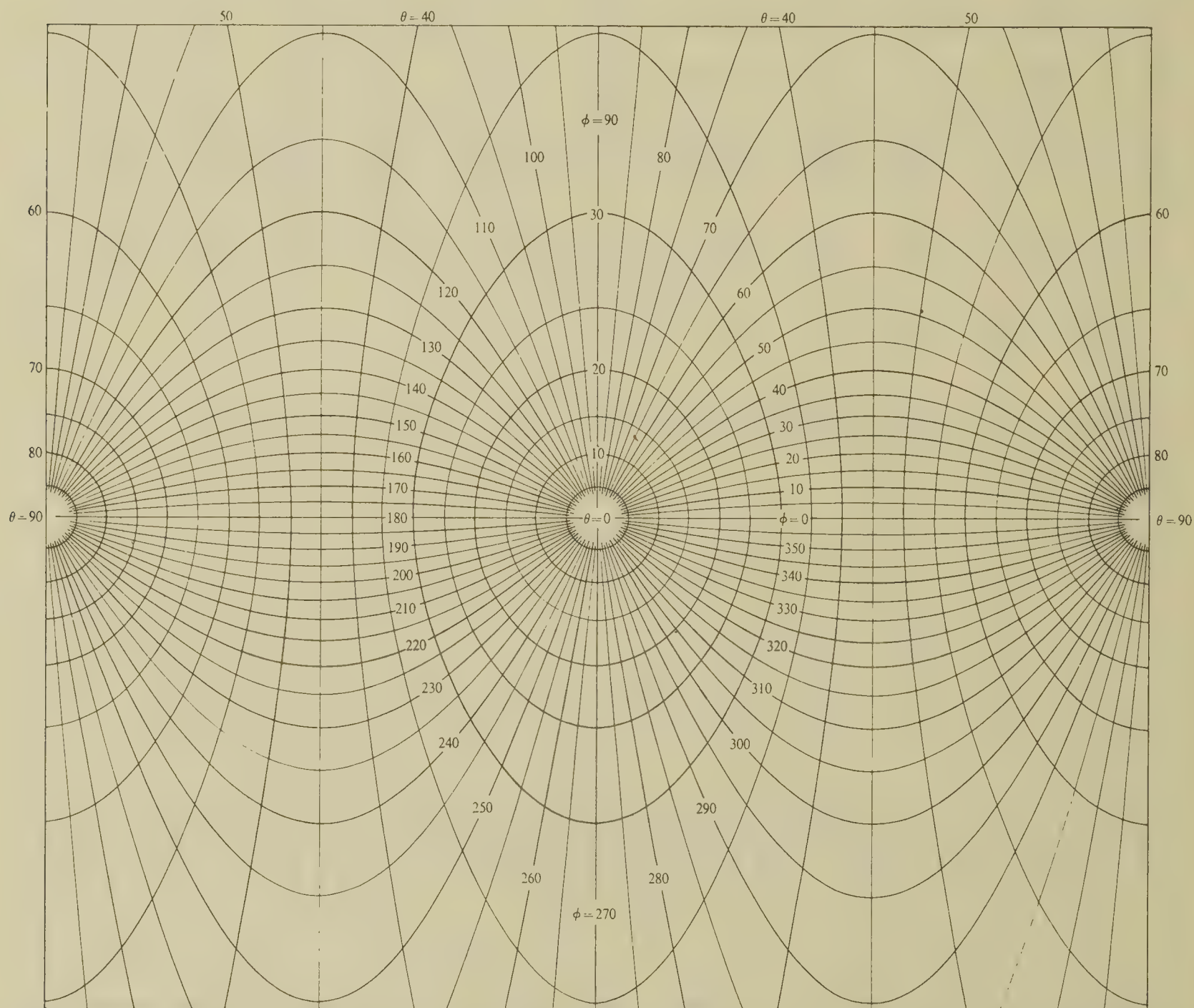


Fig. 4.2.1.2(3). Chart for Laue photo on cylindrical film: curves of θ from $90^\circ \rightarrow 0^\circ \rightarrow 90^\circ$, Φ from $0^\circ \rightarrow 180^\circ \rightarrow 360^\circ (0^\circ)$

4.3. Moving Single-crystal Methods

The interpretation of rotation and oscillation diffraction data, including those of techniques involving moving films, is best carried out in terms of the reciprocal lattice (P. P. Ewald [37], J. D. Bernal [35]) and almost always with the use of charts.

4.3.1. Symbols in Use

Since authors of different standard works have in some cases used different symbols for the same quantities, Table 4.3.1 lists the symbols used, their meanings, and the author using them in each case. Where a symbol is in fairly common usage no reference is given. The Greek alphabet is given on page 435.

TABLE 4.3.1

Symbols used to specify Quantities on Diffraction Patterns and in Reciprocal Space

- θ : Bragg angle ($\theta/2$ according to usage of von Laue [39]).
- 2θ : Angle of deviation (θ according to usage of von Laue).
- S_0 : Vector length K/λ in direction of incident beam.
- S : Vector length K/λ in direction of diffracted beam.
- σ : Reciprocal-lattice-point vector, length K/d , where d is interplanar distance (spacing) in direct space. This quantity (which must equal $S_0 - S$ for the fulfilment of the Bragg relation) is called ρ by Bernal [35], σ by Buerger [3] and d^*_{hkl} by Henry, Lipson and Wooster [9].

The constant of proportionality K (Vol. I, 2.4) (k^2 in Bernal's notation) is taken either as unity (which is more convenient in considering the Laue technique, with wavelength variable) or as λ , in which case the radius of the Ewald sphere (sphere of reflection) is unity. The latter will be assumed hereafter in this Section unless otherwise stated.

- ζ : Axial co-ordinate of reciprocal-lattice point P corresponding to any particular reflection hkl , relative to the point 000 as origin and the rotation axis as axis of cylindrical co-ordinates; that is, perpendicular distance of P from a plane normal to the rotation axis through the reciprocal-lattice origin.
- ξ : Radial co-ordinate of P ; that is, radius of a cylinder having the rotation axis as axis, and passing through P .

Lines of constant ζ on any diffraction pattern or chart are called layer lines. (Buerger, following some German authors, calls these layer lines of the 1st kind.)

Lines of constant ξ are called row lines. (Buerger refers to these as layer lines of the 2nd kind. This practice is not recommended, as it is liable to lead to confusion.)

ϕ *Rotation and Laue photographs*: The angular cylindrical co-ordinate of P measured as the acute angle between the plane containing σ and the rotation axis and the plane containing S_0 and the rotation axis. ϕ goes from $0-90^\circ$ on either side of the negative direction of S_0 . The complement of ϕ is $\bar{\phi}$. Some charts for cylindrical films are labelled ' ϕ -charts' but actually give values of $\bar{\phi}$.

Weissenberg photographs (Buerger): The angular cylindrical co-ordinate of P relative to the rotation axis and some specified direction in the crystal, normally along the positive direction of S_0 , projected on to the equatorial plane, at the beginning of the oscillation. ϕ goes from 0 to 360° . (In Bernal's notation the angular coordinate of P is ω ; Buerger uses ω for the angular rotation of a crystal corresponding to any given translation of the film holder.) The angle ϕ is sometimes referred to as τ (see Section 5.2.5.3, page 267). The axis of cylindrical co-ordinates in this case is the normal to the levels being recorded, and the origin line for τ is the horizontal axis of a precession camera.

- μ (Buerger): The angle of inclination of S_0 to the plane which is normal to the rotation axis. (Bernal's β).
- Y (Buerger): The azimuth angle of S ; that is, the angle between the projections of S_0 and S on the plane normal to the rotation axis. (Bernal's ϕ .)
- χ (Buerger): The inclination angle of S ; that is, the angle between S and its projection on the plane normal to the rotation axis ($\sin \chi = \zeta$ if $K = \lambda$. Incident beam normal to rotation axis). (In Bernal's notation this is χ also.)

ρ (Buerger): Angle between σ and the rotation axis ($\tan \rho = \xi/\zeta$). (In Bernal's notation this is α .)

ν : Angle between generator of n th layer line and the equatorial plane. ($=\chi$ for normal-beam methods.)

d^* : Interplanar distance (spacing) in reciprocal lattice.

Symbols applying to the precession method in particular are given in Section 4.5.

4.3.2. Relationships between cylindrical co-ordinates ϕ , ξ , ζ of reciprocal-lattice point P (relative to rotation axis and trace of incident beam on zero layer plane as origins), and the position of the corresponding diffraction spot, under various conditions.

4.3.2.1. GENERAL CASE

Incident beam makes angle μ with equatorial plane (normal to rotation axis). Assume $K = \lambda$.

Let ν = angle between generator of n th layer line and equatorial plane (NCR or PCM in Fig. 4.3.2.1 (a) and (c)), and Y = angle between projections of incident beam and diffracted beam on equatorial plane (A'CM).

Then $\sin \nu = \sin \mu + \zeta$ (Fig. 4.3.2.1 (a)) (1)

Diagram illustrating the geometry of a sphere of reflection. The sphere has center C and radius R . A vertical line BB' is the axis of rotation. A horizontal line AA' is the trace of the equatorial plane. An incident beam AC makes an angle μ with the trace of the equatorial plane. A point N on the sphere's surface is at a distance $\cos \nu$ from the vertical axis and $\sin \nu$ from the horizontal plane. The distance from the horizontal plane to N is ζ . The distance from the horizontal plane to the point O on the sphere's surface is $\sin \mu$. The angle between the incident beam and the radius CN is ν .

Equatorial plane

Zero layer
nth layer

Projection of incident beam

A

C

l

$\cos \mu$

R

ϕ

γ

$\cos \nu$

Q

ξ

M Projection of diffracted beam

$$\begin{aligned} \cos Y &= \frac{\cos^2 \nu + \cos^2 \mu - \xi^2}{2 \cos \nu \cos \mu} \\ &\quad (\text{Fig. 4.3.2.1 (b)}) \\ &= \frac{2 \cos^2 \mu - 2\zeta \sin \mu - \zeta^2 - \xi^2}{2 \cos \mu \sqrt{(\cos^2 \mu - 2\zeta \sin \mu - \zeta^2)}} \end{aligned} \quad \dots (2)$$

$$\begin{aligned} \cos \phi &= \frac{\cos^2 \mu + \xi^2 - \cos^2 \nu}{2\xi \cos \mu} \\ &\quad \text{(Fig. 4.3.2.1 (b))} \\ &= \frac{\zeta^2 + \xi^2 + 2\zeta \sin \mu}{2\xi \cos \mu} \quad \dots (3) \end{aligned}$$

$$\sin \nu = \zeta \quad (\text{in this case } \nu = \chi \text{ in Buerger's notation, normal beam}) \quad \dots (5)$$

176

If $\mu = +\nu$:

$\zeta = 0$ (anti-equi-inclination)

$$\cos Y = 1 - \frac{\xi^2}{2 \cos^2 \nu} \quad \dots (7)$$

If $\mu = -\nu$:

$\zeta = -2 \sin \mu = 2 \sin \nu$ (equi-inclination) $\dots (8)$

$$\cos Y = 1 - \frac{\xi^2}{2 \cos^2 \nu} \quad \dots (9)$$

If $\nu = 0$:

$\zeta = -\sin \mu$ (flat cone) $\dots (10)$

$$\cos Y = \frac{1 + \cos^2 \mu - \xi^2}{2 \cos \mu} = \frac{2 - \zeta^2 - \xi^2}{2 \sqrt{1 - \zeta^2}} \quad \dots (11)$$

In this case each layer line is brought to the equatorial position by adjustment of the direction of the incident beam so that $\mu = \sin^{-1}(-\zeta)$.

Alternatively it may be desirable to have the incident and diffracted beams always in one plane (say horizontal or vertical), the direction of the incident beam being fixed. In this case the crystal must be adjusted (e.g. by the use of an "Eulerian cradle" as described by Furnas and Harker [38]) to bring the d^* direction into the fixed plane for each reflection, the crystal and Geiger counter then being set at the appropriate θ , 2θ angles respectively.

4.3.2.3. DIFFRACTION OBSERVED ON PLANE FILM, distant D from crystal.

(a) Film parallel to rotation axis and normal to trace of incident beam on equatorial plane (Fig. 4.3.2.3(1)).

Let x , y , the co-ordinates of the diffraction spot, be measured from I, the point where the incident beam hits the film, y being parallel and x perpendicular to the rotation axis direction.

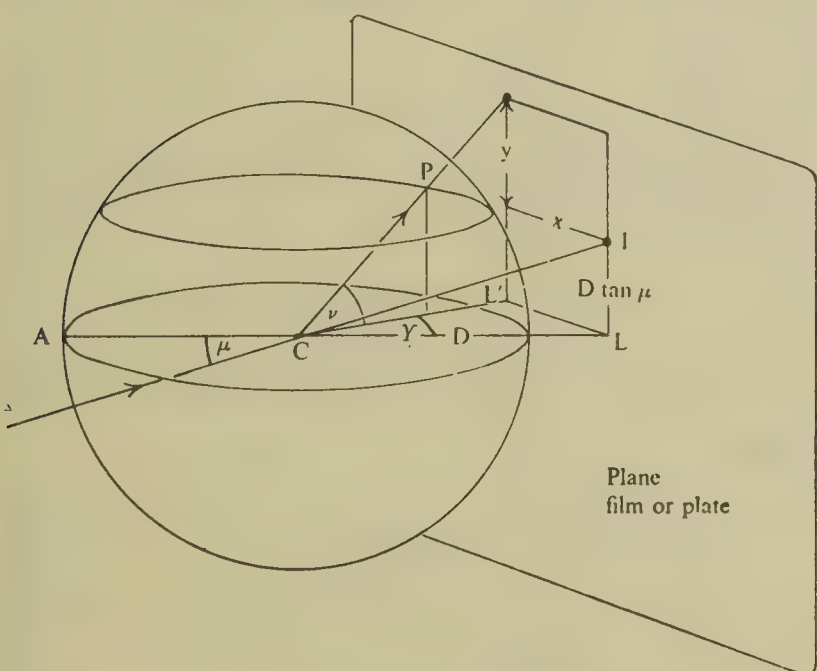


Fig. 4.3.2.3(1). Geometrical principles of photography on to plane film normal to trace of incident beam on equatorial plane. (Angle CLL' is a right angle.)

If L be the point where the trace of the incident beam hits the film, $CL = D$ and $IL = D \tan \mu$.

$$x = D \tan Y$$

$$= D \tan \cos^{-1} \frac{2 \cos^2 \mu - 2 \zeta \sin \mu - \zeta^2 - \xi^2}{2 \cos \mu \sqrt{(\cos^2 \mu - 2 \zeta \sin \mu - \zeta^2)}} \quad \dots (12)$$

$$y + D \tan \mu = D \sec Y \tan \nu$$

$$y = -D \tan \mu + \frac{2D \cos \mu (\sin \mu + \zeta)}{2 \cos^2 \mu - 2 \zeta \sin \mu - \zeta^2 - \xi^2} \quad \dots (13)$$

If $\mu = 0$:

$$x = D \tan \cos^{-1} \frac{2 - \zeta^2 - \xi^2}{2 \sqrt{1 - \zeta^2}} \quad \dots (14)$$

$$y = \frac{2D\zeta}{2 - \zeta^2 - \xi^2} \quad \dots (15)$$

(b) Film parallel to rotation axis but making angle α (CLL' in Fig. 4.3.2.3(2)) with trace of incident beam on equatorial plane. x , y measured, as before, from I, perpendicular and parallel to rotation axis.

$$x = \frac{D \sin Y}{\sin \alpha \sin (\alpha + Y)} \quad \dots (16)$$

$$y = -D \frac{\tan \mu}{\sin \alpha} + D \frac{\tan \nu}{\sin (\alpha + Y)} \quad \dots (17)$$

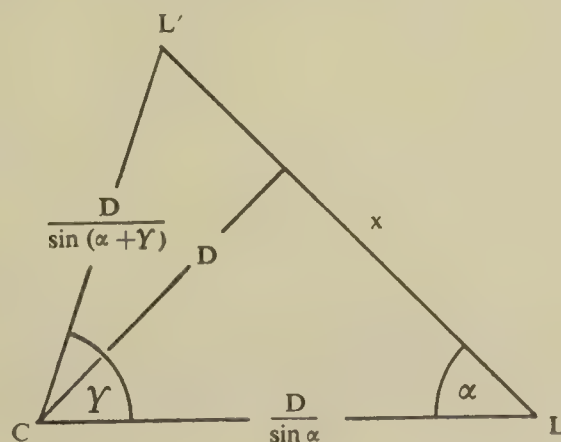


Fig. 4.3.2.3(2). Case where film makes an angle α in the equatorial plane with the trace of the incident beam.

These equations are cumbersome and would in fact seldom be necessary.

If $\mu = 0$ they reduce to:

$$x = \frac{D \sin Y}{\sin \alpha \sin (\alpha + Y)} \text{ as before,}$$

$$y = \frac{D\zeta}{\sin (\alpha + Y) \sqrt{1 - \zeta^2}} \quad \dots (18)$$

where $Y = \cos^{-1} \frac{2 - \zeta^2 - \xi^2}{2 \sqrt{1 - \zeta^2}}$ (as in (6))

If $\alpha = 90^\circ$ they reduce to (12) and (13).

4.3.2.4. CYLINDRICAL STATIONARY FILM, radius r , axis parallel to rotation axis, and incident beam inclined to equatorial plane at angle μ .

(a) *Crystal on axis of cylinder*, co-ordinates measured from point where incident beam strikes film, x round the film, y parallel to the axis (Fig. 4.3.2.4(1)).

Measuring angles in degrees:

$$x = \frac{2\pi r}{360} Y \quad \dots (19)$$

where Y is given by (2).

$$y = -r \tan \mu + r \tan \nu$$

$$= r \left(\frac{\sin \mu + \zeta}{\sqrt{(\cos^2 \mu - 2\zeta \sin \mu - \zeta^2)}} - \tan \mu \right) \quad \dots (20)$$

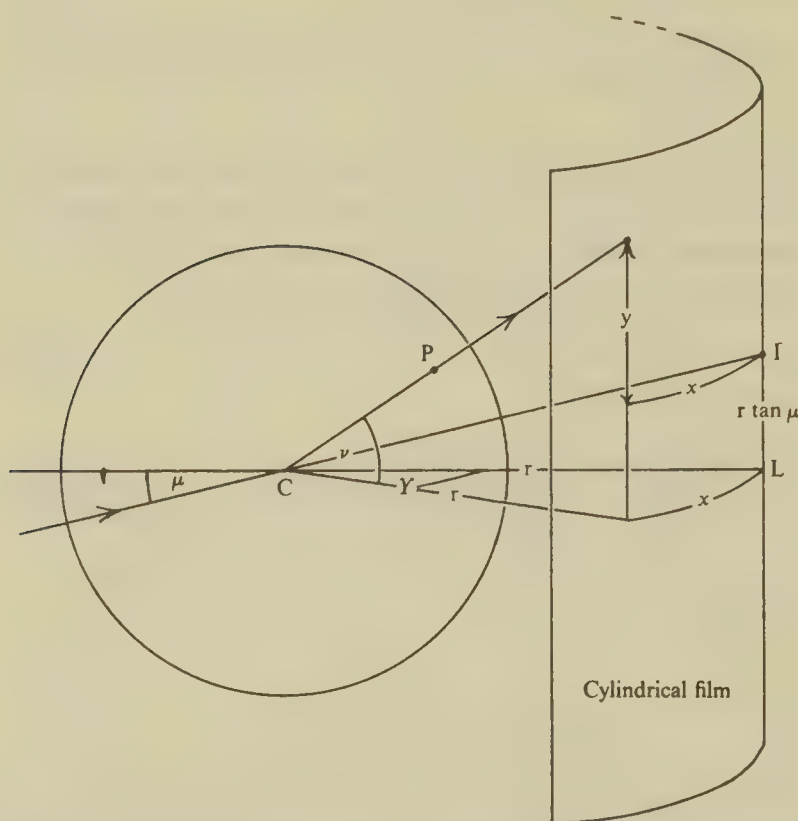


Fig. 4.3.2.4(1). Geometrical principles of photography on to a cylindrical film, axis and rotation axis of crystal coinciding. Incident beam making angle μ with equatorial plane.

If $\mu=0$: $x = \frac{2\pi r}{360} Y$ as before;

where, from (6), $\cos Y = \frac{2 - \zeta^2 - \xi^2}{2\sqrt{(1 - \zeta^2)}}$

$$y = \frac{r\zeta}{\sqrt{(1 - \zeta^2)}} \quad \dots (21)$$

(Note that Table 4.3.2 is derived from these expressions for x and y .)

If $\mu=\nu$: $y=0$

If $\mu=-\nu$: $y = 2r \tan \nu = \frac{2r\zeta}{\sqrt{(4 - \zeta^2)}} \quad \dots (22)$

The case $\mu=90^\circ$ will not normally give any diffracted beams for any one given λ .

(b) *Crystal on circumference of cylinder*. Only the case $\mu=0$ (incident beam normal to rotation axis) is of interest here, and only the zero layer line. The advantage of this method is that since the angle in a segment is constant, if the position of the source of incident radiation is fixed (at A in Fig. 4.3.2.4(2)) the position of the diffraction will occur at B where $AB=2R \sin 2\theta$ (R radius of cylinder), whatever position the crystal takes up on the circumference. A divergent beam and powdered crystal will therefore give a sharply focused diffraction line (Seemann-Bohlin method).

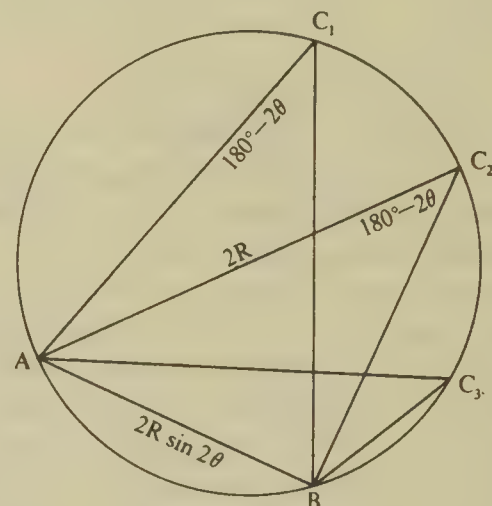


Fig. 4.3.2.4(2). Crystal on circumference of cylinder (Seemann-Bohlin method).

4.3.2.5. ALTERNATIVE EXPRESSIONS FOR ζ AND ξ

It is useful also to be able to express ζ and ξ in terms of the position of the diffraction spot: μ, ν, Y or μ, x, y .

(a) *General case*:

$$\zeta = \sin \nu - \sin \mu \quad \dots (23)$$

$$\xi = \sqrt{(\cos^2 \nu + \cos^2 \mu - 2 \cos Y \cos \nu \cos \mu)} \quad \dots (24)$$

If $\mu=0$:

$$\zeta = \sin \nu \quad \dots (25)$$

$$\xi = \sqrt{(1 + \cos^2 \nu - 2 \cos Y \cos \nu)} \quad \dots (26)$$

These expressions cover the case of diffraction measured on a *sphere*.

(b) *For a plane film*, with $\alpha=90^\circ$ (usual case):

$$\sin \nu = \sin \mu + \zeta = \frac{y + D \tan \mu}{\sqrt{\{D^2 + x^2 + (y + D \tan \mu)^2\}}} \quad \dots (27)$$

Hence

$$\zeta = \frac{y + D \tan \mu}{\sqrt{\{D^2 + x^2 + (y + D \tan \mu)^2\}}} - \sin \mu \quad \dots (28)$$

$$\xi = \sqrt{(\cos^2 \nu + \cos^2 \mu - 2 \cos Y \cos \nu \cos \mu)} \quad \dots (29)$$

where $\cos Y = \frac{D}{\sqrt{(D^2 + x^2)}}$

and $\cos^2 \nu = \frac{D^2 + x^2}{D^2 + x^2 + (y + D \tan \mu)^2}$

Hence

$$\xi = \sqrt{\left(\cos^2 \mu + \frac{D^2 + x^2 - 2D \cos \mu \sqrt{D^2 + x^2 + (y + D \tan \mu)^2}}{D^2 + x^2 + (y + D \tan \mu)^2} \right)} \quad \dots (30)$$

If $\mu=0$:

$$\zeta = \frac{y}{\sqrt{D^2 + x^2 + y^2}} \quad \dots (31)$$

$$\xi = \sqrt{\left(1 + \frac{D^2 + x^2 - 2D \sqrt{D^2 + x^2 + y^2}}{D^2 + x^2 + y^2} \right)} \quad \dots (32)$$

(c) For a cylindrical film, crystal on axis:

$$\zeta = \frac{y + r \tan \mu}{\sqrt{r^2 + (y + r \tan \mu)^2}} - \sin \mu \quad \dots (33)$$

$$\xi = \sqrt{\left\{ \cos^2 \mu + \frac{r^2}{r^2 + (y + r \tan \mu)^2} - \frac{2r \cos \mu}{\sqrt{r^2 + (y + r \tan \mu)^2}} \cos \left(\frac{360x}{2\pi r} \right) \right\}} \quad \dots (34)$$

If $\mu=0$:

$$\zeta = \frac{y}{\sqrt{r^2 + y^2}} \quad \dots (35)$$

$$\xi = \sqrt{\left\{ 1 + \frac{r^2}{r^2 + y^2} - \frac{2r}{\sqrt{r^2 + y^2}} \cos \left(\frac{360x}{2\pi r} \right) \right\}} \quad \dots (36)$$

The corresponding values of x , y , ξ , ζ have been plotted by Bernal [35] on a series of charts. The table for plotting the Bernal chart for a plane film or plate may be found in the original paper, and is not reproduced here. The charts are commercially available.

Table 4.3.2 gives data for constructing a Bernal chart for a cylindrical film, normal beam setting, radius 28.65 mm (Fig. 4.3.2.4(3)) (see 4.3.2, equations (21)).

4.3.3. Identity Distances on Stationary Films

For plane or cylindrical films, the repeat or identity period (translation t) along the rotation-axis direction $[uvw]$:

$$t(uvw) = \frac{n\lambda}{\zeta_n} \quad \dots (1)$$

(Continued on page 184)

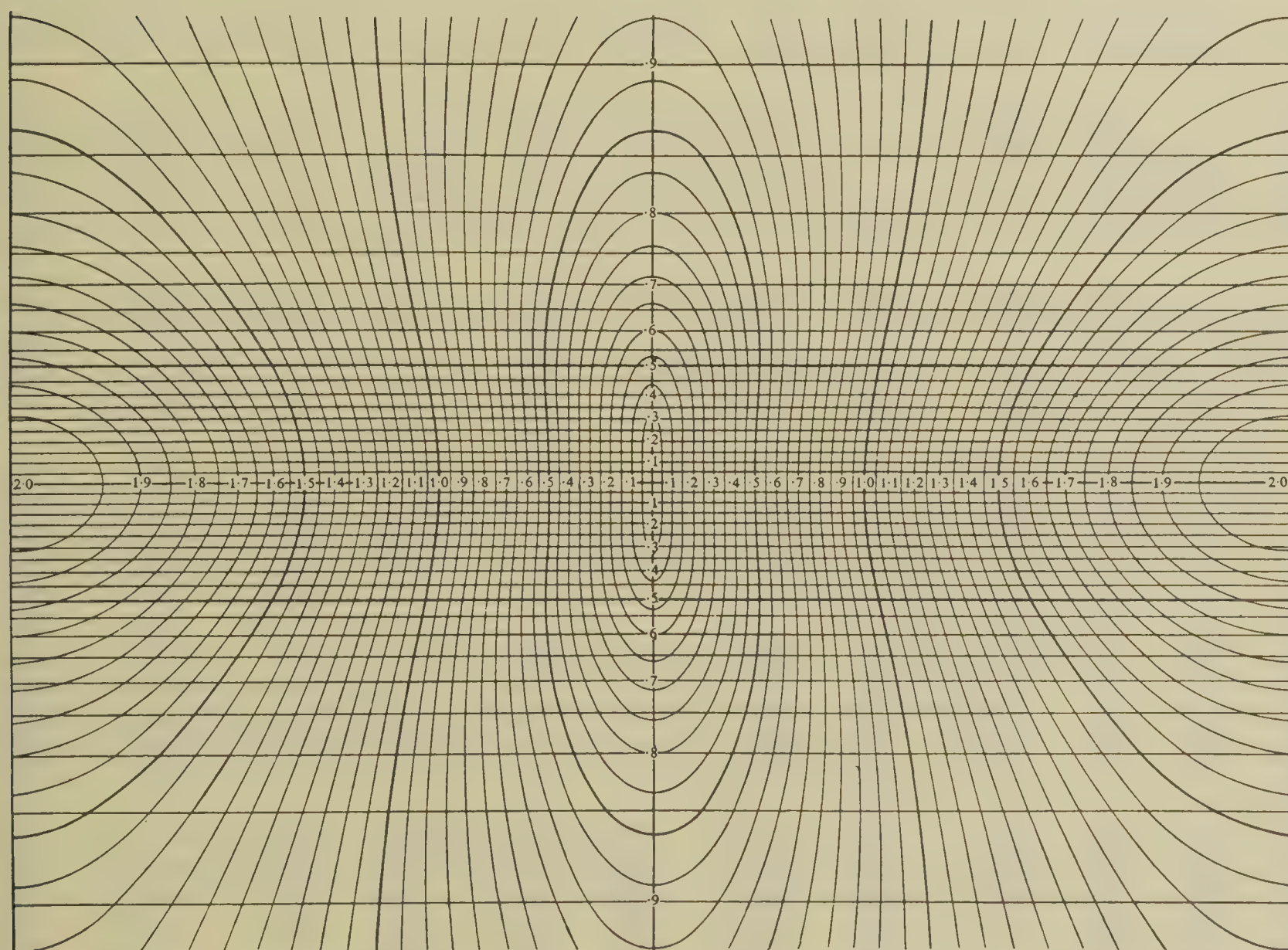


Fig. 4.3.2.4(3). Bernal chart for reading ξ and ζ co-ordinates for reflection on a rotation or oscillation photograph, cylindrical camera.

TABLE 4.3.2
Co-ordinates for Construction of Bernal Chart†

Camera radius 2.865 cm.

x = distance of point on layer line from central axis of chart in cm.
in terms of y = co-ordinate parallel to rotation axis (layer height) in cm.
and of ξ, ζ = cylindrical co-ordinates of reciprocal lattice.

For drafting purposes, the chart should be constructed to a scale magnified to 4 times or more and then reduced photographically to the scale of the table, which is that of the photograph.

ξ	$\zeta=0$ y=0	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40	0.45
		0.143	0.288	0.435	0.585	0.740	0.901	1.070	1.250	1.444
0	0									
0.05	0.143	0.143	0.143	0.140	0.132	0.113	0.057			
0.10	0.287	0.287	0.287	0.287	0.284	0.276	0.260	0.229	0.165	
0.15	0.430	0.430	0.431	0.431	0.431	0.427	0.419	0.403	0.373	0.319
0.20	0.574	0.574	0.575	0.576	0.577	0.576	0.572	0.563	0.545	0.513
0.25	0.718	0.718	0.720	0.722	0.723	0.724	0.723	0.718	0.707	0.687
0.30	0.863	0.863	0.865	0.867	0.870	0.872	0.873	0.872	0.866	0.853
0.35	1.008	1.008	1.010	1.013	1.017	1.020	1.023	1.025	1.023	1.016
0.40	1.154	1.154	1.157	1.160	1.164	1.169	1.173	1.177	1.179	1.177
0.45	1.300	1.301	1.304	1.308	1.313	1.318	1.325	1.330	1.335	1.337
0.50	1.448	1.449	1.451	1.456	1.462	1.469	1.476	1.484	1.492	1.498
0.55	1.596	1.597	1.600	1.605	1.612	1.620	1.629	1.639	1.649	1.659
0.60	1.746	1.747	1.750	1.756	1.763	1.773	1.783	1.795	1.808	1.820
0.65	1.897	1.898	1.901	1.908	1.916	1.926	1.938	1.953	1.967	1.983
0.70	2.049	2.050	2.054	2.061	2.070	2.081	2.095	2.111	2.128	2.147
0.75	2.202	2.204	2.208	2.215	2.225	2.238	2.253	2.271	2.291	2.313
0.80	2.358	2.359	2.364	2.372	2.383	2.396	2.413	2.433	2.455	2.480
0.85	2.515	2.517	2.522	2.530	2.542	2.557	2.575	2.597	2.622	2.650
0.90	2.674	2.676	2.682	2.691	2.703	2.720	2.740	2.763	2.791	2.822
0.95	2.836	2.838	2.844	2.854	2.867	2.885	2.906	2.932	2.962	2.996
1.00	3.000	3.002	3.008	3.019	3.033	3.052	3.076	3.104	3.136	3.174
1.05	3.167	3.169	3.176	3.187	3.202	3.223	3.248	3.278	3.314	3.355
1.10	3.337	3.339	3.346	3.358	3.375	3.397	3.424	3.456	3.495	3.540
1.15	3.510	3.512	3.520	3.533	3.551	3.574	3.603	3.639	3.680	3.729
1.20	3.687	3.690	3.698	3.711	3.731	3.756	3.787	3.825	3.870	3.923
1.25	3.868	3.871	3.880	3.894	3.915	3.942	3.975	4.016	4.065	4.122
1.30	4.054	4.057	4.066	4.082	4.104	4.133	4.169	4.213	4.265	4.327
1.35	4.245	4.249	4.259	4.275	4.299	4.330	4.369	4.416	4.473	4.540
1.40	4.443	4.446	4.457	4.475	4.500	4.534	4.575	4.626	4.688	4.761
1.45	4.647	4.651	4.662	4.681	4.709	4.744	4.790	4.845	4.912	4.992
1.50	4.859	4.863	4.875	4.896	4.925	4.964	5.013	5.074	5.146	5.235
1.55	5.081	5.085	5.098	5.121	5.153	5.195	5.248	5.314	5.394	5.490
1.60	5.313	5.318	5.333	5.357	5.391	5.438	5.496	5.568	5.656	5.764
1.65	5.559	5.564	5.580	5.607	5.645	5.696	5.760	5.840	5.939	6.060
1.70	5.821	5.827	5.845	5.874	5.917	5.973	6.046	6.136	6.247	6.386
1.75	6.105	6.111	6.131	6.164	6.212	6.276	6.358	6.462	6.591	6.755
1.80	6.416	6.424	6.446	6.484	6.539	6.613	6.710	6.833	6.990	7.193
1.85	6.767	6.776	6.802	6.848	6.914	7.004	7.122	7.278	7.485	7.774
1.90	7.181	7.192	7.225	7.282	7.368	7.487	7.651	7.881	8.246	
1.95	7.716	7.732	7.781	7.968	8.005	8.220	8.636			
2.00	9.000									

† Checked by I. Woodward.

For drafting purposes, the chart should be constructed to a scale magnified to 4 times or more and then reduced photographically to the scale of the table, which is that of the photograph.

TABLE 4.3.2 (continued)
Co-ordinates for Construction of Bernal Chart†
Camera radius 2.865 cm.

x = distance of point on layer line from central axis of chart in cm.
in terms of y = co-ordinate parallel to rotation axis (layer height) in cm.
and of ξ , ζ = cylindrical co-ordinates of reciprocal lattice.

ξ	$\zeta=0.50$ y=1.654	0.55	0.60	0.65	0.70	0.75	0.80	0.85	0.90	0.95
		1.887	2.149	2.451	2.808	3.249	3.820	4.623	5.915	8.717
0										
0.05										
0.10										
0.15	0.208									
0.20	0.458	0.355	0							
0.25	0.651	0.591	0.481	0.229						
0.30	0.829	0.788	0.718	0.592	0.308					
0.35	1.001	0.973	0.924	0.840	0.686	0.313				
0.40	1.168	1.150	1.117	1.057	0.953	0.753	0			
0.45	1.335	1.324	1.302	1.261	1.187	1.050	0.765			
0.50	1.500	1.497	1.484	1.457	1.405	1.307	1.117	0.639		
0.55	1.666	1.668	1.664	1.649	1.614	1.545	1.410	1.113		
0.60	1.831	1.840	1.843	1.838	1.819	1.773	1.678	1.472	0.891	
0.65	1.998	2.012	2.023	2.027	2.021	1.995	1.931	1.788	1.416	
0.70	2.166	2.185	2.202	2.216	2.221	2.213	2.177	2.081	1.829	0.670
0.75	2.336	2.360	2.384	2.405	2.422	2.430	2.417	2.363	2.198	1.553
0.80	2.507	2.537	2.566	2.596	2.624	2.646	2.657	2.638	2.544	2.145
0.85	2.681	2.714	2.750	2.789	2.827	2.864	2.896	2.911	2.879	2.655
0.90	2.857	2.895	2.938	2.984	3.033	3.084	3.136	3.183	3.208	3.129
0.95	3.035	3.079	3.128	3.182	3.241	3.307	3.379	3.457	3.537	3.590
1.00	3.217	3.266	3.321	3.384	3.454	3.534	3.627	3.736	3.871	4.051
1.05	3.402	3.457	3.519	3.589	3.671	3.767	3.880	4.022	4.212	4.523
1.10	3.592	3.652	3.721	3.800	3.894	4.005	4.141	4.316	4.566	5.019
1.15	3.786	3.851	3.928	4.017	4.123	4.251	4.410	4.622	4.937	5.556
1.20	3.985	4.057	4.141	4.240	4.360	4.505	4.691	4.944	5.334	6.163
1.25	4.189	4.268	4.361	4.472	4.605	4.771	4.986	5.285	5.765	6.906
1.30	4.401	4.487	4.590	4.713	4.862	5.050	5.298	5.652	6.250	8.079
1.35	4.620	4.715	4.827	4.964	5.132	5.346	5.634	6.058	6.826	
1.40	4.848	4.952	5.077	5.229	5.418	5.663	6.000	6.519	7.602	
1.45	5.087	5.202	5.340	5.510	5.726	6.009	6.411	7.077		
1.50	5.339	5.466	5.621	5.813	6.060	6.395	6.894	7.869		
1.55	5.607	5.748	5.923	6.144	6.434	6.842	7.516			
1.60	5.894	6.055	6.255	6.514	6.866	7.403	9.000			
1.65	6.208	6.393	6.629	6.944	7.405	8.313				
1.70	6.558	6.778	7.069	7.486	8.253					
1.75	6.964	7.241	7.638	8.386						
1.80	7.467	7.872	9.000							
1.85	8.247									
1.90										
1.95										
2.00										

† Checked by I. Woodward.

TABLE 4.3.4

Data for Bunn Chart for Indexing of Rotation Zero Line of Rectangular Lattice (see page 184)

(Scale of chart should allow 1.0 table unit = 25 cm or more)

b/a (axial ratio of net) $\log_{10}(10b/a)$	1.0 1.0 (tetragonal)	0.9 0.9542	0.8 0.9031	0.7 0.8451	0.6 0.7782	0.5773 0.7614 (hexagonal)
h, k	$2 \log_{10} \xi_0 + \text{constant} = \log_{10} 10 \left[(h^2 - k^2) \frac{(b/a)^2}{(b/a)^2 + 1} + k^2 \right] = \text{distance of points on } hk \text{ curves (Fig. 4.3.7) from reference abscissa along } b/a \text{ ordinates}$					
10	0.6990	0.6507	0.5913	0.5171	0.4228	
20	1.3010	1.2529	1.1934	1.1190	1.0249	1.0000
30	1.6532	1.6050	1.5456	1.4713	1.3770	
40	1.9031	1.8549	1.7954	1.7211	1.6269	1.6021
50			1.9893	1.9149	1.8207	
60					1.9791	1.9542
70						
80						
90						
10,0						
11,0						
12,0						
01	0.6990	0.7423	0.7852	0.8268	0.8665	
11	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
21	1.3979	1.3697	1.3365	1.2981	1.2538	
31	1.6990	1.6609	1.6151	1.5600	1.4938	1.4771
41	1.9294	1.8872	1.8353	1.7733	1.6964	
51				1.9490	1.8665	1.8451
61						
71						
81						
91						
10,1						
11,1						
02	1.3010	1.3444	1.3872	1.4288	1.4685	1.4771
12	1.3979	1.4245	1.4516	1.4790	1.5059	
22	1.6021	1.6021	1.6021	1.6021	1.6021	1.6021
32	1.8129	1.7950	1.7746	1.7516	1.7262	
42	2.0000	1.9717	1.9387	1.9002	1.8559	1.8451
52					1.9804	
62						
72						
82						
03	1.6532	1.6965	1.7394	1.7810	1.8207	
13	1.6990	1.7340	1.7692	1.8041	1.8377	1.8451
23	1.8129	1.8301	1.8481	1.8666	1.8852	
33	1.9542	1.9542	1.9542	1.9542	1.9542	1.9542
43						
04	1.9031	1.9464	1.9893			

TABLE 4.3.4 (continued)

Data for Bunn Chart for Indexing of Rotation Zero Line of Rectangular Lattice (see page 184)

(Scale of chart should allow 1.0 table unit=25 cm or more)

b/a (axial ratio of net) $\log_{10} (10b/a)$	0.5 0.6990	0.4 0.6021	0.3 0.4771	0.2 0.3010	0.1 0	0 -∞
h, k	$2 \log_{10} \xi_0 + \text{constant} = \log_{10} 10 \left[(h^2 - k^2) \frac{(b/a)^2}{(b/a)^2 + 1} + k^2 \right] = \text{distance of points on } hk \text{ curves (Fig. 4.3.7) from reference abscissa along } b/a \text{ ordinates}$					
10	0.3010	0.1396	-0.0830	-0.4150	-1.0044	-∞
20	0.9031	0.7417	0.5188	0.1870	-0.4023	-∞
30	1.2553	1.0939	0.8710	0.5392	-0.0501	-∞
40	1.5052	1.3438	1.1209	0.7892	0.1998	-∞
50	1.6990	1.5376	1.3147	0.9830	0.3936	-∞
60	1.8573	1.6960	1.4731	1.1413	0.5519	-∞
70	1.9912	1.8298	1.6070	1.2752	0.6858	-∞
80		1.9458	1.7228	1.3912	0.8018	-∞
90			1.8252	1.4935	0.9041	-∞
10,0			1.9168	1.5850	0.9956	-∞
11,0			1.9996	1.6678	1.0784	-∞
12,0				1.7434	1.1540	-∞
01	0.9031	0.9356	0.9626	0.9830	0.9957	1.0000
11	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
21	1.2041	1.1505	1.0961	1.0474	1.0127	1.0000
31	1.4150	1.3228	1.2176	1.1165	1.0331	1.0000
41	1.6021	1.4870	1.3499	1.1978	1.0599	1.0000
51	1.7634	1.6345	1.4744	1.2840	1.0925	1.0000
61	1.9031	1.7655	1.5899	1.3703	1.1292	1.0000
71		1.8820	1.6957	1.4542	1.1688	1.0000
81		1.9863	1.7925	1.5344	1.2105	1.0000
91			1.8811	1.6103	1.2533	1.0000
10,1			1.9625	1.6819	1.2967	1.0000
11,1				1.7494	1.3401	1.0000
02	1.5052	1.5376	1.5647	1.5850	1.5977	1.6021
12	1.5315	1.5547	1.5743	1.5893	1.5988	1.6021
22	1.6021	1.6021	1.6021	1.6021	1.6021	1.6021
32	1.6990	1.6711	1.6447	1.6224	1.6074	1.6021
42	1.8062	1.7524	1.6982	1.6495	1.6148	1.6021
52	1.9138	1.8386	1.7584	1.6819	1.6241	1.6021
62		1.9250	1.8223	1.7185	1.6352	1.6021
72			1.8873	1.7582	1.6479	1.6021
82			1.9520	1.7999	1.6622	1.6021
03	1.8573	1.8898	1.9168	1.9372	1.9499	1.9542
13	1.8692	1.8974	1.9211	1.9391	1.9504	1.9542
23	1.9031	1.9196	1.9339	1.9449	1.9518	1.9542
33	1.9542	1.9542	1.9542	1.9542	1.9542	1.9542
43		1.9985	1.9804	1.9670	1.9576	1.9542
04						

For the usual case ($\mu=0$ and $\alpha=90^\circ$):

$$t(uvw) = \frac{n\lambda\sqrt{(r^2+y^2)}}{y} \quad \dots (2)$$

where n is the order of the ζ_n layer line. Separate rotation photographs about crystal axes, face diagonals and a body diagonal will give the unit-cell dimensions and lattice type directly. Anomalous results may indicate that the crystal is a twin.

To give a quick measure of $t(uvw)$, a set of curves may be constructed relating t and y for $n=1, 2, \dots$ and for given values of r and λ . The measurements will not be very accurate, however, because high-order layer lines correspond to very oblique angles of interception on the film.

4.3.4. Indexing of Zero-layer Line

If the primitive translations in the reciprocal lattice normal to the rotation axis are known from rotation photographs, and goniometric information is available, from optical or Laue measurements, concerning reciprocal-lattice angles, the spots on the zero-layer line may usually be indexed directly.

Unknown primitive translations in an orthogonal zero-layer net can sometimes be determined by methods similar to those used for the powder technique (Section 4.6.2). Table 4.3.4 gives data for the construction of a Bunn chart† for indexing the orthogonal $hk0$ net on a rotation or oscillation photograph taken with $[001]$ as rotation axis.

The chart consists of discrete curves, each characterizing a particular hk combination of indices, the ordinates being

$$\log 10 \left[(h^2 - k^2) \frac{(b/a)^2}{(b/a)^2 + 1} + k^2 \right]$$

and the abscissae b/a (Fig. 4.3.4) or preferably $\log(10b/a)$; the factor 10 merely being a constant which avoids most negative quantities in the table.

This chart is used in conjunction with a paper ruler, on which are recorded the *observed* $2 \log \xi_0$ values for all zero-layer line reflections ($\xi_0 = 2 \sin \theta$, where $\theta = (180/2\pi)(x/r)$, in degrees, for a cylindrical film; $\theta = \frac{1}{2} \tan^{-1}(x/D)$ for a plane film).

This ruler is drawn to the same scale as the chart ordinates, which are based on the equation

$$\xi_0^2 = h^2 a^{*2} + k^2 b^{*2} = \lambda^2 \left[\frac{1}{a^2} + \frac{1}{b^2} \right] \left[(h^2 - k^2) \frac{(b/a)^2}{(b/a)^2 + 1} + k^2 \right]$$

$$\text{Hence } 2 \log \xi_0 = \log \frac{\lambda^2}{10} \left[\frac{1}{a^2} + \frac{1}{b^2} \right]$$

$$+ \log 10 \left[(h^2 - k^2) \frac{(b/a)^2}{(b/a)^2 + 1} + k^2 \right]$$

$$\text{or } 2 \log \xi_0 + C = \log 10 \left[(h^2 - k^2) \frac{(b/a)^2}{(b/a)^2 + 1} + k^2 \right]$$

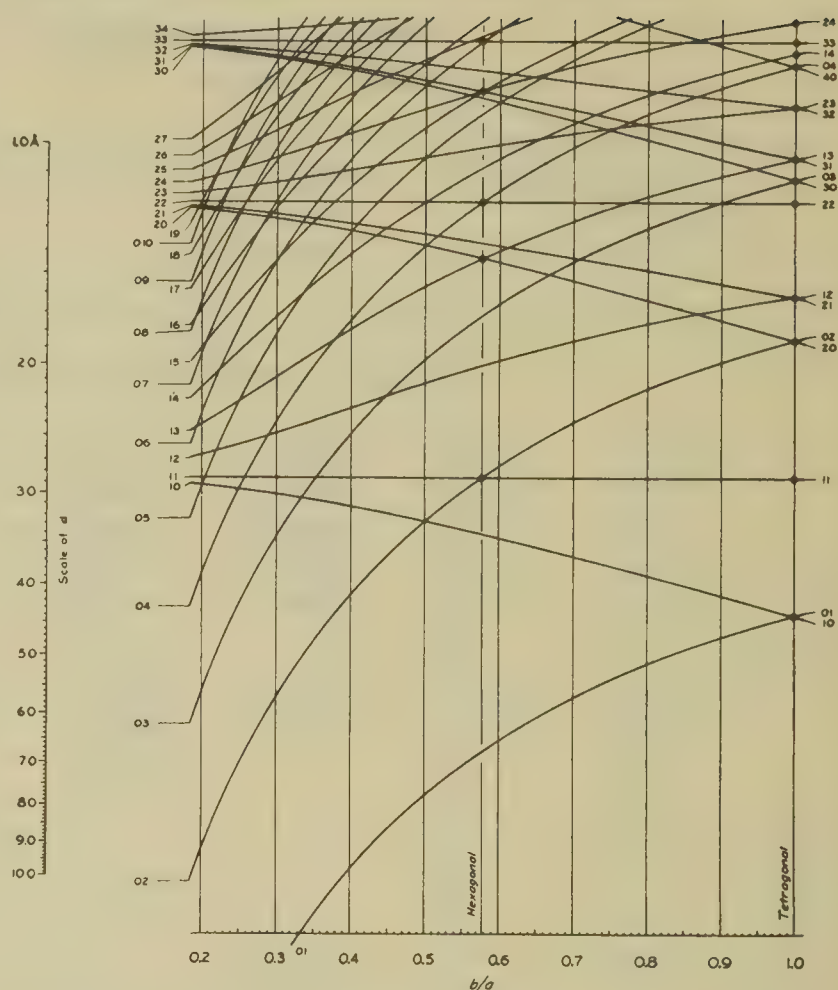


Fig. 4.3.4. Bunn chart for indexing an orthogonal net from the zero row of a rotation photograph.

The value of C , which is unknown, is independent of h, k and is taken care of by being able to move the paper ruler, which is kept parallel to the ordinate axis, not only (1) along the b/a axis, but also (2) normal to the b/a axis (thus changing $2 \log \xi_0$ into $2 \log \xi_0 + C$), until a match is found for a particular value of b/a , after which the h, k values can be read off the chart (Fig. 4.3.4 and [5], page 142).

This chart assumes $a > b$, but can of course also be used for $a < b$ by interchanging h and k .

The chart can only be applied with accuracy if drawn on a large scale and if sharp and accurately measurable reflections are available.

Using a Bernal chart of suitable scale, reflections on higher-layer lines can usually be indexed by inspection.

The oscillation method does not require separate tables and is described in references [9] and [35].

If the reciprocal-lattice nets are not orthogonal, a moving-film method will give axial angles as well as lengths.

† The construction and use of this chart are described by C. W. Bunn on pages 132–35, 142–43 and Appendix 3 of his *Chemical Crystallography* [5]. The following misprints should, however, be noted in earlier editions of the book:

Page 380, last line: MX should be XN/MN.

Page 381, lines 24 and 27: $1/a^2$ in numerator should be $1/c^2$; line 33: $MX = 4/3a^2 \div (\dots)$ should be $MX/MN = 1/c^2 \div (\dots)$; last line: $4/3a^2$ in numerator should be $1/c^2$.

4.4. Weissenberg Method

4.4.1. Experimental Details

The principles of this technique are very adequately described by M. J. Buerger [3]. Three arrangements are in common use.

(a) *Normal-beam*. X-ray beam perpendicular to crystal rotation axis. Screens adjusted to record only one layer line (constant ζ) for any one exposure. Crystal usually oscillated through about 200° .

Using Buerger's notation (Table 4.3.1), $\mu = \mu_N = 0$.

(b) *Equi-inclination*. X-ray beam inclined at angle $\mu = \mu_E$, such that it lies on the cone generator for the given ζ level.

Using Buerger's notation, $\mu_E = -\nu$.

This method doubles the range of the reciprocal lattice that can be recorded, using successive n -layer-line photographs.

(c) *Flat-cone*. X-ray beam inclined to plane normal to the rotation axis at an angle μ_F , such that the ζ level desired emerges in an equatorial plane normal to the rotation axis.

Using Buerger's notation, $\nu = 0$.

Table 4.4.1A gives μ_E and layer-line screen setting s_E for the equi-inclination method, in terms of ζ , for a Weissenberg camera diameter $2r = 5.73$ cm, having screens of diameter $2r_s = 5$ cm.

$$s_E = r_s \tan \mu_E = r_s \frac{\zeta}{\sqrt{4 - \zeta^2}}. \text{ That is, } \zeta = 2 \sin \mu_E.$$

Table 4.4.1B gives setting constants $\mu_F (= \sin^{-1} \zeta)$ for the flat-cone method ($s_F = 0$), and $s_N = \{r_s \tan \nu = r_s \zeta / \sqrt{1 - \zeta^2}\}$ for the normal-beam method ($\mu_N = 0$), for a range of values of ζ , and corresponding values of y_{rot} , the height in cm of the layer line on a rotation photograph; for the same size camera $\{y = r \zeta / \sqrt{1 - \zeta^2}\}$.

Appropriate factors must be applied for cameras of other dimensions.

4.4.2. Interpretation of Weissenberg Patterns

In order to construct the reciprocal lattice from a Weissenberg pattern it is necessary to determine the cylindrical co-ordinates ξ and ϕ (Table 4.3.1) from the $x_W y_W$ co-ordinates measured on the film in mm (ζ being known and constant for the given pattern).

First consider the instrumental constants C_1, C_2 of the camera. C_1 depends on the camera diameter and is the ratio of the reflection angle $Y (= 2\theta)$ for the zero layer line of a normal-beam pattern, to the x_W co-ordinate measured round the film from the incident-beam trace as origin. $C_1 = Y/x_W$.

In general, $C_1 = 360/2\pi r$.

If $2r = 5.73$ cm, $C_1 = 2^\circ/\text{mm}$, $x_W = Y/2$.

C_2 is the ratio of the crystal rotation ω to the corresponding traverse of the camera y_W and is generally also $2^\circ/\text{mm}$.

A central row of the pattern is then inclined at $\tan^{-1} 2 = 63^\circ 26'$ to the y direction (direction of traverse).

y_W is measured from a central row as origin line. In terms of x_W, y_W and μ_E , ξ and ϕ have the following values:

$$\xi = 2 \sin x_W \cos \mu_E \quad \dots (1)$$

$$\phi = C_2 y_W \quad \dots (2)$$

A nomogram for the determination of ξ is shown in Figure 4.4.2(1), and Table 4.4.2A gives data for its construction.

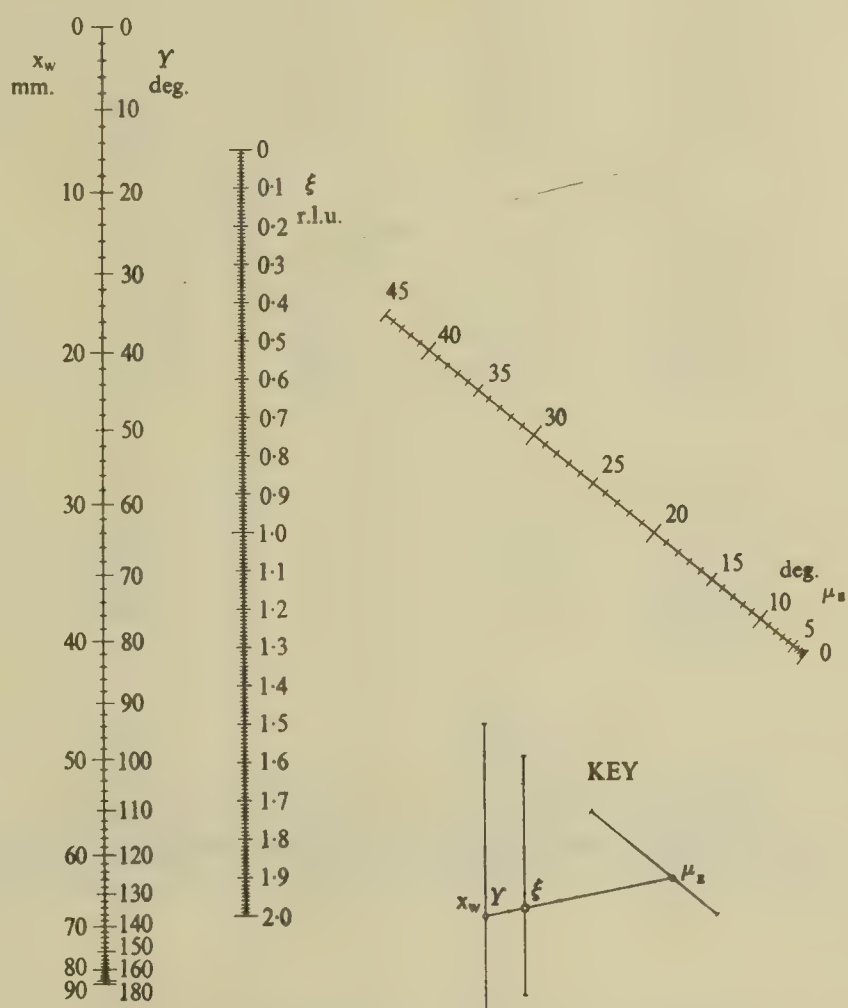


Fig. 4.4.2(1). Nomogram for transforming Weissenberg film co-ordinates to cylindrical reciprocal-lattice co-ordinates.

Buerger ([3]; see pages 261–68) has described a convenient method involving scales and measuring devices for determining ξ and ϕ directly for each spot, but greater accuracy is obtained by the use of standard millimetre scales and measuring instruments. If care is taken to maintain the film truly cylindrical in the film holder, a precision of 0.3% can be expected for ordinary Weissenberg methods. Precision can be greatly increased either by the use of a calibrating pattern (e.g. Ag powder pattern on edge of film, [36]), or by the provision of special Straumanis film arrangements (Buerger [3], Chapter 21).

Weissenberg patterns of known lattices are indexed

4.4. WEISSENBERG METHOD

directly for the determination of symmetry or listing intensities. Sketches of the indexed Weissenberg patterns on transparent overlays are very useful in this connection. A template showing a series of equally spaced row lines in the reciprocal-lattice plane transformed to Weissenberg co-ordinates (for the above-mentioned camera dimensions) is reproduced full size in Fig. 4.4.2(2). Buerger has given a table for the con-

struction of this chart on Cartesian co-ordinates, but the work is greatly simplified if points on the curves are laid off from the zero line along axes parallel to the central row line (at an angle of $63^{\circ} 26'$ for the previously described camera arrangement). Table 4.4.2B gives these distances for row lines at equal intervals of 0.10 r.l.u., for axes erected at equal intervals of $\bar{\phi}$ (5° or 2.5 mm) along the zero row line.

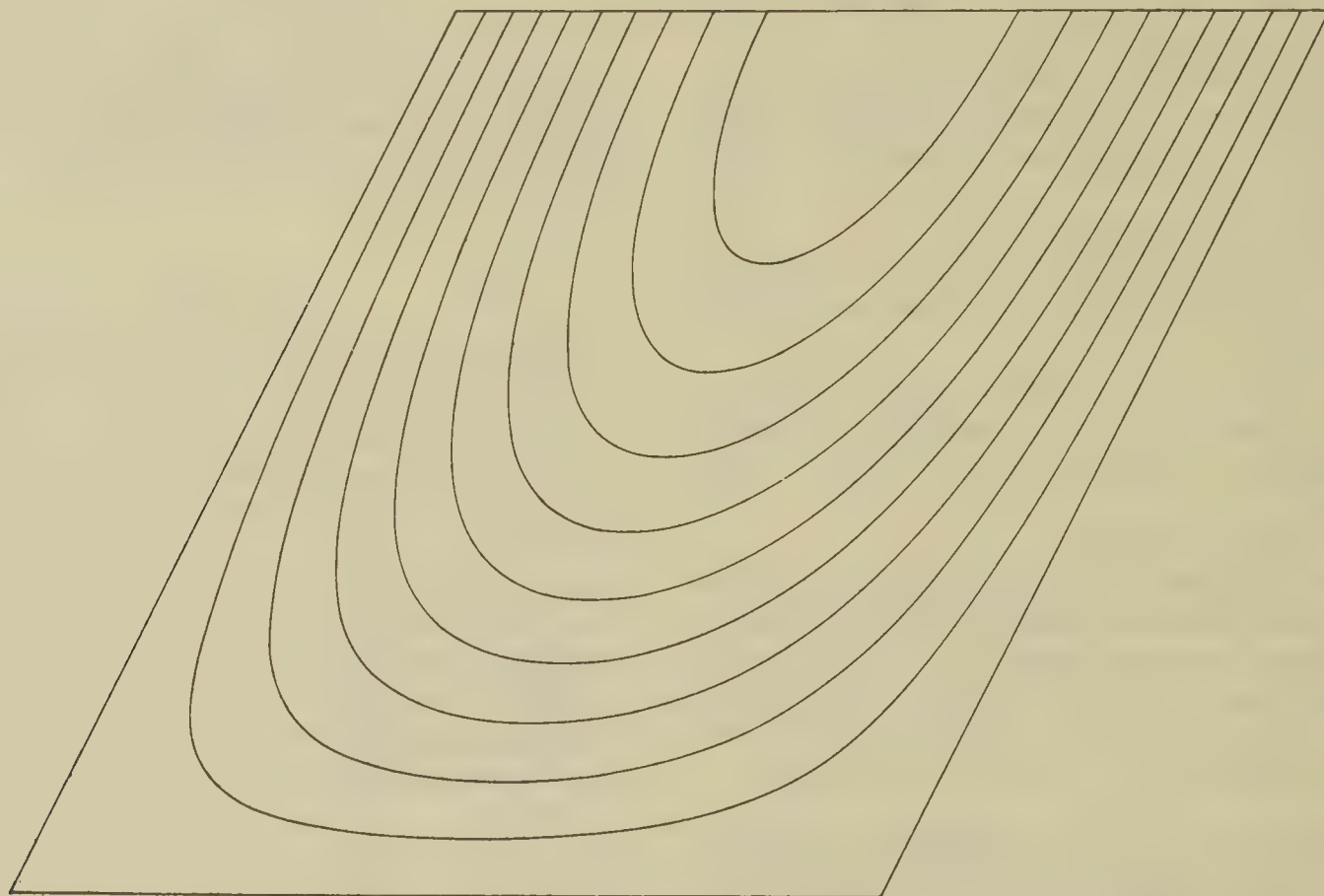


Fig. 4.4.2(2). Equi-inclination Weissenberg transform of parallel lattice rows. With the bottom line of the chart placed on the trace of the direct beam, and the sloping sides along a chosen central lattice row, the curves show the apparent shape of a set of lattice rows parallel to the central row.

4.4. WEISSENBERG METHOD

TABLE 4.4.1A
Equi-inclination Weissenberg Method Setting Constants

Camera diameter = 5.73 cm

Screen diameter = 5.00 cm

ζ = layer height in reciprocal-lattice units

μ_E = camera-inclination angle

s_E = layer-line screen setting (cm)

ζ	μ_E	s_E (cm)	ζ	μ_E	s_E (cm)	ζ	μ_E	s_E (cm)
0.00	0° 00'	0	0.35	10° 05'	0.444	0.70	20° 29'	0.934
0.01	0 17	0.013	0.36	10 22	0.458	0.71	20 48	0.949
0.02	0 34	0.025	0.37	10 40	0.471	0.72	21 06	0.965
0.03	0 52	0.038	0.38	10 57	0.484	0.73	21 25	0.980
0.04	1 09	0.050	0.39	11 15	0.497	0.74	21 43	0.996
0.05	1° 26'	0.063	0.40	11° 32'	0.510	0.75	22° 02'	1.011
0.06	1 43	0.075	0.41	11 50	0.524	0.76	22 20	1.027
0.07	2 00	0.088	0.42	12 07	0.537	0.77	22 39	1.043
0.08	2 18	0.100	0.43	12 25	0.550	0.78	22 57	1.059
0.09	2 35	0.113	0.44	12 43	0.564	0.79	23 16	1.075
0.10	2° 52'	0.125	0.45	13° 00'	0.577	0.80	23° 35'	1.091
0.11	3 09	0.138	0.46	13 18	0.591	0.81	23 54	1.107
0.12	3 26	0.150	0.47	13 36	0.604	0.82	24 12	1.123
0.13	3 44	0.163	0.48	13 53	0.618	0.83	24 31	1.140
0.14	4 01	0.175	0.49	14 11	0.632	0.84	24 50	1.157
0.15	4° 18'	0.188	0.50	14° 29'	0.645	0.85	25° 09'	1.174
0.16	4 35	0.201	0.51	14 46	0.659	0.86	25 28	1.191
0.17	4 53	0.213	0.52	15 04	0.673	0.87	25 47	1.208
0.18	5 10	0.226	0.53	15 22	0.687	0.88	26 06	1.225
0.19	5 27	0.238	0.54	15 40	0.701	0.89	26 25	1.242
0.20	5° 44'	0.251	0.55	15° 58'	0.715	0.90	26° 45'	1.260
0.21	6 02	0.264	0.56	16 16	0.729	0.91	27 04	1.277
0.22	6 19	0.277	0.57	16 34	0.743	0.92	27 23	1.295
0.23	6 36	0.289	0.58	16 51	0.758	0.93	27 43	1.313
0.24	6 54	0.302	0.59	17 09	0.772	0.94	28 02	1.331
0.25	7° 11'	0.315	0.60	17° 27'	0.786	0.95	28° 22'	1.350
0.26	7 28	0.328	0.61	17 46	0.801	0.96	28 41	1.368
0.27	7 46	0.341	0.62	18 04	0.815	0.97	29 01	1.387
0.28	8 03	0.353	0.63	18 22	0.830	0.98	29 20	1.405
0.29	8 20	0.366	0.64	18 40	0.844	0.99	29 40	1.424
0.30	8° 38'	0.379	0.65	18° 58'	0.859	1.00	30° 00'	1.443
0.31	8 55	0.392	0.66	19 16	0.874	1.01	30 20	1.463
0.32	9 12	0.405	0.67	19 34	0.889	1.02	30 40	1.482
0.33	9 30	0.418	0.68	19 52	0.904	1.03	31 00	1.502
0.34	9 47	0.431	0.69	20 11	0.919	1.04	31 20	1.522

4.4. WEISSENBERG METHOD

TABLE 4.4.1A (continued)

ζ	μ_E	s_E (cm)	ζ	μ_E	s_E (cm)	ζ	μ_E	s_E (cm)
1.05	31° 40'	1.542	1.20	36° 52'	1.875	1.35	42° 27'	2.287
1.06	32 00	1.562	1.21	37 14	1.900	1.36	42 51	2.319
1.07	32 21	1.583	1.22	37 35	1.925	1.37	43 14	2.351
1.08	32 41	1.604	1.23	37 57	1.950	1.38	43 38	2.383
1.09	33 01	1.625	1.24	38 19	1.976	1.39	44 02	2.417
1.10	33° 22'	1.646	1.25	38° 41'	2.002			
1.11	33 43	1.668	1.26	39 03	2.028			
1.12	34 03	1.690	1.27	39 25	2.055			
1.13	34 24	1.712	1.28	39 48	2.083			
1.14	34 45	1.734	1.29	40 10	2.110			
1.15	35° 06'	1.757	1.30	40° 33'	2.138			
1.16	35 27	1.780	1.31	40 55	2.167			
1.17	35 48	1.803	1.32	41 18	2.196			
1.18	36 09	1.827	1.33	41 41	2.226			
1.19	36 31	1.851	1.34	42 04	2.256			

4.4. WEISSENBERG METHOD

TABLE 4.4.1B

Normal-beam and Flat-cone Weissenberg Methods Setting Constants

Camera diameter = 5.73 cm

Screen diameter = 5.00 cm

 ζ = layer height in reciprocal-lattice units y_{rot} = layer height (cm) on rotation film from same camera μ_F = camera-inclination angle for flat-cone method ($s_F=0$) s_N = layer-line screen setting (cm) for normal-beam method ($\mu_N=0$)

ζ	y_{rot} (cm)	μ_F	s_N (cm)	ζ	y_{rot} (cm)	μ_F	s_N (cm)
0.00	0	0	0	0.35	1.071	20° 29'	0.934
0.01	0.029	0° 34'	0.025	0.36	1.105	21 06	0.965
0.02	0.057	1 09	0.050	0.37	1.141	21 43	0.996
0.03	0.086	1 43	0.075	0.38	1.177	22 20	1.027
0.04	0.115	2 18	0.100	0.39	1.213	22 57	1.059
0.05	0.143	2° 52'	0.125	0.40	1.250	23° 35'	1.091
0.06	0.172	3 26	0.150	0.41	1.288	24 12	1.124
0.07	0.201	4 01	0.175	0.42	1.326	24 50	1.157
0.08	0.230	4 35	0.201	0.43	1.365	25 28	1.191
0.09	0.259	5 10	0.226	0.44	1.404	26 06	1.225
0.10	0.288	5° 44'	0.251	0.45	1.444	26° 45'	1.260
0.11	0.317	6 19	0.277	0.46	1.484	27 23	1.295
0.12	0.346	6 54	0.302	0.47	1.525	28 02	1.331
0.13	0.376	7 28	0.328	0.48	1.568	28 41	1.368
0.14	0.405	8 03	0.353	0.49	1.610	29 20	1.405
0.15	0.435	8° 38'	0.379	0.50	1.654	30° 00'	1.443
0.16	0.464	9 12	0.405	0.51	1.699	30 40	1.482
0.17	0.494	9 47	0.431	0.52	1.744	31 20	1.521
0.18	0.524	10 22	0.457	0.53	1.791	32 00	1.562
0.19	0.554	10 57	0.484	0.54	1.838	32 41	1.604
0.20	0.585	11° 32'	0.510	0.55	1.887	33° 22'	1.646
0.21	0.615	12 07	0.537	0.56	1.937	34 03	1.690
0.22	0.646	12 43	0.564	0.57	1.988	34 45	1.735
0.23	0.677	13 18	0.591	0.58	2.040	35 27	1.780
0.24	0.708	13 53	0.618	0.59	2.094	36 09	1.827
0.25	0.740	14° 29'	0.646	0.60	2.149	36° 52'	1.875
0.26	0.771	15 04	0.673	0.61	2.206	37 35	1.925
0.27	0.803	15 40	0.701	0.62	2.264	38 19	1.976
0.28	0.836	16 16	0.729	0.63	2.324	39 03	2.029
0.29	0.868	16 51	0.758	0.64	2.386	39 48	2.083
0.30	0.901	17° 27'	0.786	0.65	2.451	40° 33'	2.138
0.31	0.934	18 04	0.815	0.66	2.517	41 18	2.195
0.32	0.968	18 40	0.844	0.67	2.586	42 04	2.256
0.33	1.002	19 16	0.874	0.68	2.657	42 51	2.318
0.34	1.036	19 52	0.904	0.69	2.731	43 38	2.383

4.4. WEISSENBERG METHOD

TABLE 4.4.2A

Data for Nomogram for Conversion of Equi-inclination Weissenberg Film Co-ordinates to Reciprocal-lattice Cylindrical Co-ordinates

For layout see Fig. 4.4.2(1). Tabulated figures give a convenient scale for drafting, but the chart may be reduced photographically for use. x_W, y_W Weissenberg film co-ordinates. x, y co-ordinates on nomogram.

A. Scale for film co-ordinate, x_W . Origin at 0-0; scale extends vertically downward to $x=0, y=-45$ cm.

x_W (cm)	y Scale (cm)	x_W (cm)	y Scale (cm)	x_W (cm)	y Scale (cm)
0	0	3.0	22.47	6.0	38.97
0.1	0.79	3.1	23.16	6.1	39.36
0.2	1.58	3.2	23.84	6.2	39.73
0.3	2.36	3.3	24.51	6.3	40.10
0.4	3.14	3.4	25.16	6.4	40.45
0.5	3.92	3.5	25.81	6.5	40.78
0.6	4.70	3.6	26.45	6.6	41.11
0.7	5.48	3.7	27.08	6.7	41.42
0.8	6.26	3.8	27.71	6.8	41.72
0.9	7.04	3.9	28.32	6.9	42.01
1.0	7.81	4.0	28.93	7.0	42.29
1.1	8.59	4.1	29.52	7.1	42.55
1.2	9.36	4.2	30.11	7.2	42.80
1.3	10.13	4.3	30.69	7.3	43.03
1.4	10.89	4.4	31.26	7.4	43.25
1.5	11.65	4.5	31.82	7.5	43.46
1.6	12.40	4.6	32.37	7.6	43.66
1.7	13.16	4.7	32.91	7.7	43.85
1.8	13.91	4.8	33.44	7.8	44.01
1.9	14.65	4.9	33.96	7.9	44.17
2.0	15.39	5.0	34.47	8.0	44.32
2.1	16.13	5.1	34.97	8.1	44.45
2.2	16.86	5.2	35.46	8.2	44.56
2.3	17.58	5.3	35.94	8.3	44.66
2.4	18.30	5.4	36.41	8.4	44.75
2.5	19.02	5.5	36.86	8.5	44.83
2.6	19.72	5.6	37.30	8.6	44.89
2.7	20.43	5.7	37.74	8.7	44.94
2.8	21.13	5.8	38.16	8.8	44.97
2.9	21.82	5.9	38.57	8.9	44.99
				9.0	45.00

4.4. WEISSENBERG METHOD

TABLE 4.4.2A (continued)

B. Scale for inclination setting, μ_E . Origin at $x=33$ cm, $y=-30$ cm; scale extends diagonally upward and left towards 0-0, the origin of scale A.

μ_E (deg.)	Scale (cm)	μ_E (deg.)	Scale (cm)	μ_E (deg.)	Scale (cm)
0	0	15	5.62	30	16.35
1	0.03	16	6.28	31	17.04
2	0.11	17	6.97	32	17.72
3	0.26	18	7.66	33	18.38
4	0.45	19	8.38	34	19.03
5	0.70	20	9.10	35	19.66
6	1.00	21	9.83	36	20.30
7	1.36	22	10.57	37	20.91
8	1.75	23	11.30	38	21.51
9	2.20	24	12.04	39	22.08
10	2.68	25	12.77	40	22.64
11	3.21	26	13.51	41	23.20
12	3.77	27	14.23	42	23.73
13	4.36	28	14.94	43	24.27
14	4.98	29	15.64	44	24.78
				45	25.29

C. Scale for radial reciprocal-lattice co-ordinate, ξ . Origin at $x=7.20$ cm, $y=-6.55$ cm (on line of scale B extended); scale extends vertically downward to $y=-41.75$ cm. Scale marked for intervals of ξ of 0.01 from 0 to 2.00, at equal intervals of y of 0.176 cm.

TABLE 4.4.2B

Data for Row-line Indexing Chart for Weissenberg Equi-inclination Photographs

For layout see Fig. 4.4.2(2). For drafting purposes the chart should be constructed to a scale magnified to 5 times or more, then reduced photographically to the scale of the table.

Entries are distances in cm from base (x axis) along axes parallel to zero row-line ($d^*=0$) (inclination angle $63^\circ 26'$). Coupling ratio: 1 mm/2 deg.; camera diameter: 5.73 cm ($r_F=2.86$ cm). d^* is in reciprocal-lattice units. Table entries are $0.01951 \times 2.86Y$, where $\sin(Y/2)=d^*/2 \sin \bar{\phi}$.

$\bar{\phi} =$ $x =$	0° 0 (cm)	5° 0.25	10° 0.50	15° 0.75	20° 1.00	25° 1.25	30° 1.50	35° 1.75	40° 2.00	45° 2.25	50° 2.50
d^* (r.l.u.)											
0	0-10.063	0	0	0	0	0	0	0	0	0	0
0.1		3.913	1.872	1.246	0.940	0.759	0.642	0.559	0.499	0.454	0.418
0.2			3.931	2.541	1.901	1.531	1.290	1.122	1.001	0.908	0.839
0.3			6.680	3.960	2.908	2.324	1.952	1.695	1.508	1.370	1.263
0.4				5.657	4.002	3.159	2.636	2.282	2.027	1.837	1.692
0.5				8.385	5.251	4.054	3.354	2.889	2.559	2.316	2.130
0.6					6.854	5.056	4.122	3.526	3.110	2.806	2.578
0.7						6.251	4.968	4.204	3.688	3.317	3.040
0.8						7.957	5.940	4.944	4.302	3.852	3.520
0.9							7.173	5.778	4.968	4.419	4.023
1.0							10.063	6.782	5.709	5.031	4.556
1.1								8.219	6.576	5.709	5.131
1.2									7.711	6.489	5.765
1.3										7.471	6.490
1.4										9.154	7.383
1.5											8.749
1.6											
1.7											
1.8											
1.9											
2.0											

4.4. WEISSENBERG METHOD

TABLE 4.4.2B (continued)

Column on right gives values of x for $Y=180^\circ$, for the values of d^* given on the left.

$\bar{\phi} =$ $x =$	55° 2.75	60° 3.00	65° 3.25	70° 3.50	75° 3.75	80° 4.00	85° 4.25	90° 4.50	
d^* (r.l.u.)									x ($Y=180^\circ$)
0	0	0	0	0	0	0	0	0	0
0.1	0.391	0.370	0.353	0.341	0.332	0.325	0.322	0.321	0.143
0.2	0.784	0.741	0.708	0.683	0.664	0.652	0.644	0.642	0.287
0.3	1.180	1.115	1.066	1.027	0.998	0.979	0.968	0.965	0.431
0.4	1.580	1.493	1.426	1.375	1.336	1.310	1.295	1.290	0.577
0.5	1.987	1.876	1.790	1.726	1.677	1.645	1.625	1.619	0.724
0.6	2.403	2.266	2.161	2.083	2.023	1.983	1.960	1.952	0.873
0.7	2.829	2.665	2.540	2.446	2.376	2.328	2.300	2.291	1.024
0.8	3.268	3.076	2.928	2.819	2.735	2.680	2.646	2.636	1.179
0.9	3.725	3.500	3.328	3.201	3.104	3.040	3.002	2.990	1.337
1.0	4.206	3.942	3.743	3.597	3.485	3.411	3.369	3.354	1.500
1.1	4.718	4.407	4.177	4.008	3.881	3.796	3.747	3.731	1.668
1.2	5.266	4.903	4.635	4.440	4.293	4.197	4.140	4.122	1.843
1.3	5.872	5.437	5.124	4.897	4.728	4.619	4.554	4.533	2.027
1.4	6.564	6.029	5.654	5.388	5.192	5.065	4.991	4.968	2.221
1.5	7.412	6.707	6.244	5.926	5.694	5.546	5.461	5.433	2.429
1.6	8.675	7.544	6.929	6.531	6.251	6.073	5.973	5.940	2.656
1.7		8.826	7.793	7.250	6.891	6.671	6.548	6.508	2.910
1.8			9.308	8.207	7.681	7.385	7.224	7.173	3.208
1.9					8.895	8.354	8.104	8.029	3.590
2.0								10.063	4.500

4.5. Buerger Precession Method

The Buerger precession camera (Buerger [3]) registers layers of the reciprocal lattice in true shape. The camera is prepared for a photograph by means of various settings: $\bar{\mu}$, inclination of crystal translation to X-ray beam; r_s , layer-screen annular radius; s , screen-to-crystal distance setting; Fd^* , upper-level film setting (F is the crystal-to-film axis setting, d^* the upper-level height). They are related by the expression

$$s = r_s \cot \cos^{-1}(\cos \bar{\mu} - d^*) \quad \dots (1)$$

For the common case where $d^*=0$ (zero-level photography), equation (1) reduces to

$$s = r_s \cot \bar{\mu} \quad \dots (2)$$

Table 4.5.1 gives screen settings s for zero-level photographs as given by equation (2), for two practical choices of screen radius r_s , 15 and 20 mm. For upper levels, Table 4.5.2 gives the trigonometric part of equation (1), and these values must be multiplied by the chosen screen radius to yield the screen setting, s . Care must be exercised to select a screen radius (and inclination angle) which will not cause the screen to interfere with the film holder on the camera.

TABLE 4.5.1
Layer-screen Settings for Zero-level Photographs with the Buerger Precession Camera

Table values give screen setting s in mm; screen radius r_s is in mm.

$\bar{\mu}$ (deg.)	$r_s=15$	$r_s=20$
20	41.2	
21	39.1	
22	37.1	
23	35.3	
24	33.7	
25	32.2	42.9
26	30.8	41.0
27	29.4	39.3
28	28.2	37.6
29	27.1	36.1
30	26.0	34.6

When a film in an envelope is inserted in the screen holder, the pattern obtained from an oriented crystal consists of a concentric series of circles of spots ("cone-axis" photograph), corresponding to the various upper levels parallel to the film. The radii of

the circles, r_l , are related to the level height d^* by equation (1) by replacing r_s with r_l . Table 4.5.3 may be used to convert r_l readings in mm to d^* values in reciprocal-lattice units, providing screen-to-crystal distance s is fixed at 40.0 mm.

$$d^* = \cos \bar{\mu} - \{s/\sqrt{(r_l^2 + s^2)}\} \quad \dots (3)$$

All of the settings and transformations based on equation (1) may be conveniently determined from a nomogram given in Fig. 4.5.4, which is modified from Adams and Evans [40]. Table 4.5.4 gives data for the construction of this nomogram.

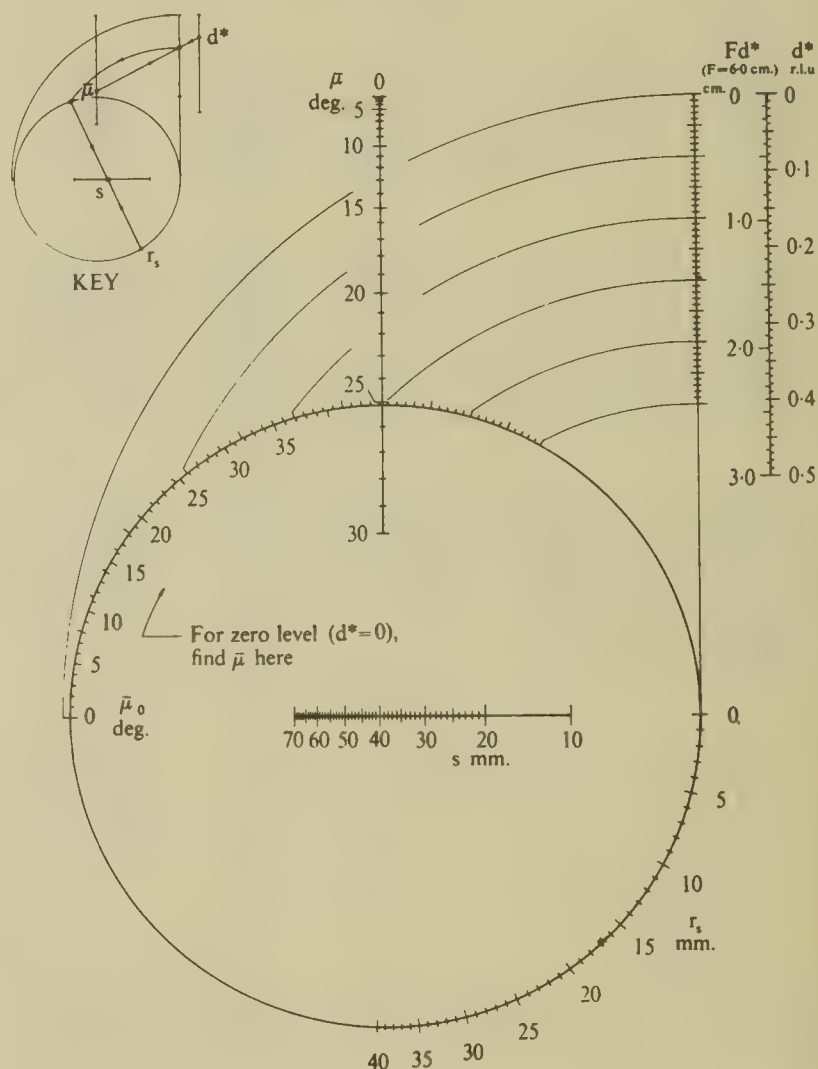


Fig. 4.5.4. Nomogram for determination of setting constants of the Buerger precession camera for photographing a given lattice plane.

A valuable application of the precession instrument is made in the orientation of crystals. Fig. 4.5.5 shows the appearance of a mis-set zero-level plane with error angle less than $\bar{\mu}$ in (a) and greater than $\bar{\mu}$ in (b). The direction of displacement of the zero-level trace permits the tilt error to be associated with one or both of the setting arcs of the goniometer head or the spindle dial. Let the difference of the distances (in mm) from the centre of the pattern to the opposite edges of the trace in the direction of displacement be called $F\Delta$,

(Continued on page 198)

TABLE 4.5.2

Data for setting the Buerger Precession Camera for Upper Levels

Screen setting s is given in mm by multiplying tabulated values by screen radius r_s in mm. (See equation 4.5(1).)
 Fd^* given in mm for $F=60.0$ mm.

d^* (r.l.u.) Fd^* (mm)	0	0.01	0.02	0.03	0.04	0.05	0.06	0.07	0.08
	0	0.60	1.20	1.80	2.40	3.00	3.60	4.20	4.80
$\bar{\mu}$ (deg.)									
15	3.732	3.257	2.915	2.658	2.452	2.282	2.140	2.017	1.910
16	3.487	3.084	2.788	2.556	2.368	2.213	2.080	1.965	1.865
17	3.271	2.926	2.665	2.459	2.289	2.145	2.022	1.914	1.819
18	3.077	2.783	2.552	2.365	2.210	2.078	1.963	1.862	1.774
19	2.904	2.649	2.444	2.276	2.135	2.012	1.906	1.812	1.728
20	2.748	2.524	2.343	2.190	2.061	1.949	1.850	1.762	1.683
21	2.605	2.408	2.246	2.109	1.990	1.887	1.795	1.712	1.638
22	2.475	2.302	2.156	2.031	1.922	1.827	1.741	1.664	1.594
23	2.356	2.203	2.072	1.957	1.857	1.769	1.689	1.617	1.552
24	2.246	2.109	1.990	1.886	1.795	1.712	1.638	1.571	1.509
25	2.145	2.022	1.914	1.819	1.734	1.658	1.589	1.525	1.467
26	2.050	1.939	1.841	1.754	1.676	1.606	1.541	1.481	1.426
27	1.963	1.862	1.774	1.693	1.620	1.555	1.494	1.438	1.387
28	1.881	1.789	1.708	1.634	1.567	1.505	1.449	1.396	1.347
29	1.804	1.721	1.646	1.578	1.516	1.458	1.405	1.355	1.309
30	1.732	1.656	1.587	1.523	1.466	1.412	1.362	1.315	1.272
d^* (r.l.u.) Fd^* (mm)	0.09	0.10	0.11	0.12	0.13	0.14	0.15	0.16	0.17
	5.40	6.00	6.60	7.20	7.80	8.40	9.00	9.60	10.20
$\bar{\mu}$ (deg.)									
15	1.816	1.731	1.656	1.586	1.523	1.465	1.412	1.361	1.315
16	1.775	1.695	1.622	1.556	1.495	1.439	1.387	1.339	1.294
17	1.734	1.658	1.589	1.525	1.467	1.413	1.363	1.317	1.273
18	1.693	1.620	1.555	1.494	1.438	1.387	1.338	1.293	1.250
19	1.652	1.584	1.520	1.462	1.409	1.360	1.313	1.269	1.228
20	1.611	1.546	1.486	1.431	1.380	1.332	1.287	1.245	1.205
21	1.571	1.509	1.452	1.399	1.350	1.304	1.261	1.221	1.182
22	1.531	1.472	1.418	1.367	1.320	1.276	1.235	1.196	1.159
23	1.491	1.435	1.384	1.336	1.291	1.248	1.209	1.171	1.136
24	1.452	1.399	1.350	1.304	1.261	1.221	1.182	1.146	1.112
25	1.413	1.363	1.317	1.273	1.232	1.193	1.156	1.121	1.088
26	1.375	1.328	1.283	1.242	1.202	1.165	1.130	1.096	1.064
27	1.338	1.293	1.250	1.211	1.173	1.138	1.104	1.071	1.040
28	1.302	1.259	1.218	1.180	1.144	1.110	1.077	1.046	1.017
29	1.266	1.225	1.186	1.150	1.116	1.082	1.051	1.022	0.993
30	1.231	1.192	1.155	1.120	1.088	1.056	1.026	0.997	0.970

4.5. BUERGER PRECESSION METHOD

TABLE 4.5.2 (continued)

d^* (r.l.u.) Fd^* (mm)	0.18 10.80	0.19 11.40	0.20 12.00	0.21 12.60	0.22 13.20	0.23 13.80	0.24 14.40	0.25 15.00	0.26 15.60
$\bar{\mu}$ (deg.)									
15	1.271	1.230	1.191	1.155	1.120	1.087	1.056	1.025	0.997
16	1.251	1.212	1.174	1.138	1.104	1.072	1.041	1.011	0.984
17	1.232	1.193	1.156	1.121	1.088	1.057	1.027	0.998	0.970
18	1.211	1.173	1.138	1.104	1.071	1.040	1.011	0.983	0.956
19	1.190	1.153	1.118	1.086	1.054	1.024	0.996	0.968	0.942
20	1.168	1.133	1.099	1.067	1.036	1.007	0.979	0.952	0.927
21	1.146	1.112	1.079	1.048	1.018	0.990	0.963	0.937	0.911
22	1.124	1.091	1.059	1.029	1.000	0.973	0.946	0.920	0.896
23	1.102	1.070	1.039	1.010	0.982	0.955	0.929	0.904	0.880
24	1.079	1.048	1.018	0.990	0.963	0.937	0.911	0.887	0.863
25	1.057	1.027	0.998	0.970	0.944	0.918	0.894	0.870	0.847
26	1.034	1.005	0.977	0.950	0.924	0.900	0.876	0.853	0.830
27	1.011	0.983	0.956	0.930	0.905	0.881	0.858	0.835	0.813
28	0.988	0.961	0.935	0.910	0.886	0.862	0.840	0.818	0.796
29	0.966	0.939	0.914	0.889	0.866	0.843	0.821	0.800	0.779
30	0.943	0.917	0.893	0.869	0.847	0.824	0.803	0.782	0.762

d^* (r.l.u.) Fd^* (mm)	0.27 16.20	0.28 16.80	0.29 17.40	0.30 18.00	0.31 18.60	0.32 19.20	0.33 19.80	0.34 20.40	0.35 21.00
$\bar{\mu}$ (deg.)									
15	0.969	0.943	0.917	0.893	0.869	0.846	0.824	0.803	0.782
16	0.957	0.931	0.906	0.882	0.858	0.836	0.813	0.793	0.772
17	0.944	0.918	0.894	0.870	0.847	0.824	0.803	0.783	0.763
18	0.930	0.905	0.881	0.858	0.835	0.814	0.792	0.772	0.752
19	0.916	0.892	0.868	0.845	0.823	0.802	0.781	0.761	0.741
20	0.902	0.878	0.855	0.832	0.811	0.790	0.769	0.749	0.730
21	0.887	0.864	0.841	0.819	0.798	0.777	0.757	0.738	0.719
22	0.872	0.849	0.827	0.805	0.784	0.761	0.745	0.725	0.707
23	0.857	0.834	0.812	0.791	0.771	0.751	0.732	0.713	0.695
24	0.841	0.819	0.798	0.777	0.757	0.738	0.719	0.700	0.682
25	0.825	0.804	0.783	0.763	0.743	0.724	0.705	0.687	0.669
26	0.809	0.788	0.767	0.748	0.728	0.710	0.692	0.674	0.657
27	0.792	0.772	0.752	0.733	0.714	0.696	0.679	0.660	0.643
28	0.776	0.756	0.736	0.717	0.699	0.681	0.664	0.647	0.630
29	0.759	0.740	0.721	0.702	0.684	0.667	0.649	0.633	0.616
30	0.742	0.723	0.705	0.686	0.669	0.652	0.635	0.618	0.603

4.5. BUERGER PRECESSION METHOD

TABLE 4.5.3

Reciprocal-lattice Layer Heights from Cone-axis Photographs with the Buerger Precession Camera

Screen-to-crystal distance, $s=40.0$ mmTable values give d^* for upper level in reciprocal-lattice units (equation 4.5(3))Radius of trace of upper level, r , given in mm

r (mm)	$\mu=5^\circ$	10°	15°	r (mm)	$\mu=5^\circ$	10°	15°
0	<div>Zero-layer circle: r_0 (mm)= 3.50 7.05 10.72</div>			35	0.244	0.232	0.213
1				36	0.253	0.241	0.223
2				37	0.262	0.251	0.232
3				38	0.271	0.260	0.241
4	0.001			39	0.280	0.269	0.250
5	0.004			40	0.289	0.278	0.259
6	0.007			41	0.298	0.286	0.268
7	0.011			42	0.307	0.295	0.276
8	0.016	0.004		43	0.315	0.304	0.285
9	0.021	0.009		44	0.323	0.312	0.293
10	0.026	0.015		45	0.332	0.320	0.302
11	0.032	0.021	0.002	46	0.340	0.329	0.310
12	0.038	0.027	0.008	47	0.348	0.336	0.318
13	0.045	0.034	0.015	48	0.356	0.344	0.326
14	0.052	0.041	0.022	49	0.364	0.353	0.334
15	0.060	0.048	0.030	50	0.371	0.360	0.341
16	0.068	0.056	0.037	51	0.379	0.368	0.349
17	0.076	0.065	0.046	52	0.387	0.375	0.356
18	0.084	0.073	0.054	53	0.394	0.383	0.364
19	0.093	0.082	0.063	54	0.401	0.390	0.371
20	0.102	0.090	0.072	55	0.408	0.397	0.378
21	0.111	0.099	0.081	56	0.415	0.404	0.385
22	0.120	0.109	0.090	57	0.422	0.411	0.392
23	0.129	0.118	0.099	58	0.428	0.417	0.398
24	0.139	0.127	0.108	59	0.435	0.424	0.405
25	0.148	0.137	0.118	60	0.441	0.430	0.411
26	0.158	0.146	0.128	61	0.448	0.436	0.417
27	0.167	0.156	0.137	62	0.454	0.443	0.424
28	0.177	0.166	0.147	63	0.460	0.449	0.430
29	0.187	0.175	0.156	64	0.466	0.455	0.436
30	0.196	0.185	0.166	65	0.472	0.461	0.442
31	0.206	0.194	0.176	66	0.478	0.467	0.448
32	0.215	0.204	0.185	67	0.484	0.472	0.453
33	0.224	0.213	0.194	68	0.489	0.478	0.459
34	0.234	0.223	0.204	69	0.495	0.483	0.464
				70	0.500	0.489	0.470

4.5. BUERGER PRECESSION METHOD

so that for the horizontal goniometer-head arc and the dial:

$$F\Delta_{\text{arc}} = x_{\text{Rt}} - x_{\text{Lt}}$$

$$F\Delta_{\text{dial}} = y_{\text{Up}} - y_{\text{Dn}}$$

(For the case of Fig. 4.5.5 (b), y_{Dn} is negative.) The corresponding angle of tilt ϵ is given by

$$\Delta = \frac{\sin 4\epsilon \cos \bar{\mu}}{\cos^2 2\epsilon - \sin^2 \bar{\mu}} \quad \dots (4)$$

Table 4.5.5 gives the setting error ϵ in terms of Δ and $F\Delta$ for the customary film-to-crystal distance $F=60$ mm. If the goniometer-head arcs are not approximately parallel and perpendicular to the film, ϵ_{arc} must be resolved between the two arcs.

Table 4.5.6 gives setting constants for the de-Jong and Bouman method. (Buerger [3], chapter 17.)

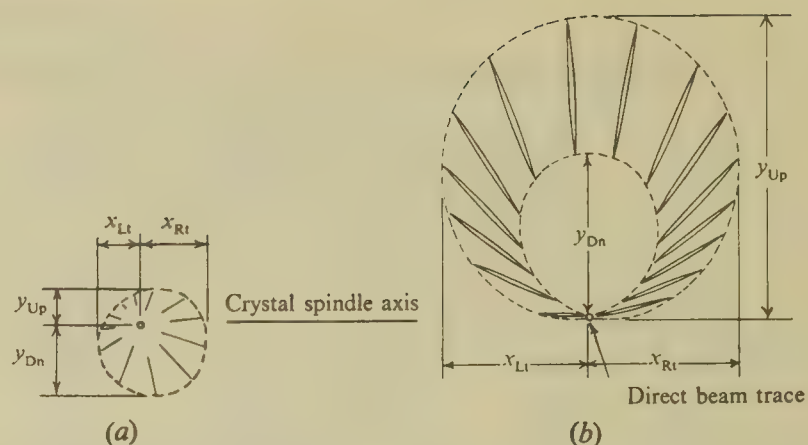


Fig. 4.5.5. Appearance of disoriented zero-level lattice plane on Buerger precession orientation photograph: (a) $\bar{\mu}=5^\circ$, arc error and dial error about 1° ; (b) $\bar{\mu}=5^\circ$, no arc error, dial error about 20° ($x_{\text{Rt}}=x_{\text{Lt}}$; y_{Dn} is negative).

TABLE 4.5.4

Data for Construction of Buerger Precession Setting Nomogram (Fig. 4.5.4)

Tabulated figures are based on a circle 30 cm in diameter, a convenient scale for drafting; the chart may be reduced photographically for use.

A. r_s scale, lower semicircle, origin at right. Circle diameter, 30 cm.

r_s (mm)	deg.	r_s (mm)	deg.	r_s (mm)	deg.	r_s (mm)	deg.	r_s (mm)	deg.	r_s (mm)	deg.
0	0	10	$28^\circ 56'$	20	$54^\circ 36'$	25	$65^\circ 39'$	30	$75^\circ 28'$	35	$84^\circ 10'$
1	$2^\circ 58'$	11	$31^\circ 42'$	21	$56^\circ 54'$	26	$67^\circ 42'$	31	$77^\circ 18'$	36	$85^\circ 46'$
2	$5^\circ 55'$	12	$34^\circ 24'$	22	$59^\circ 10'$	27	$69^\circ 44'$	32	$79^\circ 06'$	37	$87^\circ 20'$
3	$8^\circ 52'$	13	$37^\circ 06'$	23	$61^\circ 22'$	28	$71^\circ 42'$	33	$80^\circ 50'$	38	$88^\circ 52'$
4	$11^\circ 48'$	14	$39^\circ 44'$	24	$63^\circ 32'$	29	$73^\circ 36'$	34	$82^\circ 36'$	39	$90^\circ 22'$
5	$14^\circ 42'$	15	$42^\circ 19'$							40	$91^\circ 48'$
6	$17^\circ 36'$	16	$44^\circ 52'$								
7	$20^\circ 28'$	17	$47^\circ 22'$								
8	$23^\circ 20'$	18	$49^\circ 50'$								
9	$26^\circ 08'$	19	$52^\circ 14'$								

B. s scale, horizontal diameter, origin at right.

s (mm)	Scale (cm)	s (mm)	Scale (cm)	s (mm)	Scale (cm)	s (mm)	Scale (cm)	s (mm)	Scale (cm)	s (mm)	Scale (cm)
0	0	25	11.769	35	14.241	45	16.122	55	17.604	65	18.798
10	6.156	26	12.051	36	14.451	46	16.287	56	17.736	66	18.906
20	10.215	27	12.324	37	14.658	47	16.446	57	17.862	67	19.011
21	10.548	28	12.588	38	14.859	48	16.605	58	17.988	68	19.113
22	10.869	29	12.846	39	15.051	49	16.755	59	18.111	69	19.215
23	11.178	30	13.095	40	15.243	50	16.908	60	18.231	70	19.314
24	11.478	31	13.338	41	15.426	51	17.052	61	18.351		
		32	13.572	42	15.606	52	17.193	62	18.465		
		33	13.803	43	15.783	53	17.334	63	18.579		
		34	14.025	44	15.957	54	17.469	64	18.690		

4.5. BUERGER PRECESSION METHOD

TABLE 4.5.4 (continued)

C. $\bar{\mu}_0$ scale, for zero level settings only; inside upper semicircle, given in degrees measured from origin at right. $\bar{\mu}_0$ interval 1 degree, linear scale interval 2 deg.: $\bar{\mu}_0=0$, scale=180 deg., to $\bar{\mu}_0=35$ deg., scale=110 deg.

D. x scale (transfer from scale E along arcs); outside upper semicircle, origin at right.

x	Scale (deg.)	x	Scale (deg.)	x	Scale (deg.)	x	Scale (deg.)	x	Scale (deg.)	x	Scale (deg.)
1.00	180° 00'	0.90	128° 19'	0.80	106° 12'	0.70	88° 52'	0.60	73° 44'	0.50	60° 00'
0.99	163 47	0.89	125 45	0.79	104 22	0.69	87 16	0.59	72 19		
0.98	157 02	0.88	123 17	0.78	102 32	0.68	85 44	0.58	70 54		
0.97	151 52	0.87	120 55	0.77	100 42	0.67	84 08	0.57	69 30		
0.96	147 30	0.86	118 38	0.76	98 56	0.66	82 36	0.56	68 08		
0.95	143° 36'	0.85	116° 26'	0.75	97° 10'	0.65	81° 05'	0.55	66° 44'		
0.94	140 06	0.84	114 17	0.74	95 28	0.64	79 35	0.54	65 22		
0.93	136 52	0.83	112 12	0.73	93 46	0.63	78 06	0.53	64 00		
0.92	133 51	0.82	110 10	0.72	92 06	0.62	76 38	0.52	62 40		
0.91	131 00	0.81	108 12	0.71	90 28	0.61	75 10	0.51	61 20		

E. x scale (arbitrary units); vertical scale extending up from origin at right end of horizontal diameter on circle. x runs from 0.50 at $y_{sc}=15.00$ cm to 1.00 at $y_{sc}=30.00$ cm, at x intervals of 0.01, corresponding to linear scale intervals of 0.30 cm.

F. $\bar{\mu}$ scale, extending vertically along line through centre of circle ($x_{sc}=-15.00$ cm). $\bar{\mu}$ runs from 0 deg. at $y_{sc}=30.00$ cm to 30 deg. at $y_{sc}=8.796$.

$\bar{\mu}$	Scale (cm)	$\bar{\mu}$	Scale (cm)	$\bar{\mu}$	Scale (cm)	$\bar{\mu}$	Scale (cm)	$\bar{\mu}$	Scale (cm)	$\bar{\mu}$	Scale (cm)
0°	30.000	5°	29.399	10°	27.595	15°	24.603	20°	20.457	25°	15.174
1	29.968	6	29.130	11	27.088	16	23.877	21	19.494	26	13.986
2	29.905	7	28.813	12	26.535	17	23.085	22	18.480	27	12.753
3	29.779	8	28.465	13	25.950	18	22.263	23	17.421	28	11.472
4	29.620	9	28.054	14	25.299	19	21.375	24	16.314	29	10.158
										30°	8.796

G. d^* scale, extending vertically along line parallel and to right of scale E ($x_{sc}=3.41$ cm). d^* (right side of scale) runs from 0.00 r.l.u. at $y_{sc}=30.00$ cm to 0.50 r.l.u. at $y_{sc}=11.50$ cm, at d^* intervals of 0.01 r.l.u., corresponding to linear scale intervals of 0.370 cm.

H. Fd^* scale, for $F=6.00$ cm, coincident with scale G. Fd^* (left side of scale) runs from 0 mm at $y_{sc}=30.00$ cm to 30 mm at $y_{sc}=11.50$ cm at intervals of 1 mm with linear scale intervals of 0.617 cm.

4.5. BUERGER PRECESSION METHOD

TABLE 4.5.5

Angular Setting Error in Terms of Displacement of Zero-level Lattice Plane on the Buerger Precession Photograph

 Δ = displacement in reciprocal-lattice units; $F = 6.00$ cm, film-to-crystal distance; μ = camera-inclination angle. Table entries = ϵ , angular correction to appropriate goniometer arc (see text, equation 4.5(4), and Fig. 4.5.5).

$F\Delta$ (cm)	Δ (r.l.u.)	μ					
		5°	10°	15°	20°	25°	30°
0	0	0	0	0	0	0	0
0.1	0.0167	0° 14'	0° 14'	0° 14'	0° 13'	0° 13'	0° 12'
0.2	0.0333	0 28	0 28	0 27	0 26	0 25	0 24
0.3	0.0500	0 43	0 42	0 41	0 40	0 38	0 36
0.4	0.0667	0 57	0 56	0 55	0 53	0 51	0 48
0.5	0.0833	1° 11'	1° 10'	1° 09'	1° 07'	1° 05'	1° 02'
0.6	0.1000	1 25	1 24	1 23	1 21	1 18	1 14
0.7	0.1167	1 39	1 38	1 36	1 33	1 30	1 26
0.8	0.1333	1 53	1 52	1 50	1 47	1 44	1 39
0.9	0.1500	2 05	2 06	2 04	2 00	1 56	1 51
1.0	0.1667	2° 21'	2° 20'	2° 18'	2° 14'	2° 10'	2° 04'
1.1	0.1833	2 35	2 34	2 32	2 28	2 24	
1.2	0.2000	2 49	2 47	2 44	2 39	2 34	
1.3	0.2167	3 03	3 01	2 58	2 52	2 47	
1.4	0.2333	3 17	3 15	3 12	3 06	3 00	
1.5	0.2500	3° 31'	3° 29'	3° 26'	3° 20'	3° 13'	
1.6	0.2667	3 45	3 43	3 40	3 33		
1.7	0.2833	3 59	3 56	3 52	3 44		
1.8	0.3000	4 13	4 10	4 06	3 58		
1.9	0.3167	4 27	4 24	4 20	4 11		
2.0	0.3333	4° 41'	4° 38'	4° 34'	4° 25'		
2.1	0.3500	4 55	4 52	4 47			
2.2	0.3667	5 09	5 05	5 00			
2.3	0.3833	5 23	5 19	5 14			
2.4	0.4000	5 37	5 33	5 27			
2.5	0.4167	5° 51'	5° 47'	5° 41'			
2.6	0.4333	6 05	6 01				
2.7	0.4500	6 19	6 15				
2.8	0.4667	6 33	6 28				
2.9	0.4833	6 47	6 42				
3.0	0.5000	7° 00'	6° 55'				

4.5. BUERGER PRECESSION METHOD

TABLE 4.5.6

De Jong and Bouman Method Setting Constants

Fixed level-cone angle, $\nu=45^\circ$. $\sin \mu = \sin \nu - \zeta$ ($\sin \nu = 1/\sqrt{2}$). $\Delta = (D \cos \mu)/\sin \nu$ ζ = layer height in reciprocal-lattice units y_{rot} = layer height (cm) from rotation pattern (camera diameter 5.73 cm) μ = camera-inclination angle Δ_0 = film rotation-axis displacement (film-to-crystal distance $D=1$ cm) Δ = ditto for $D=3$ cm

ζ (r.l.u.)	y_{rot} (cm)	μ (deg.)	Δ_0 $D=1$ cm	Δ $D=3.0$ cm	ζ (r.l.u.)	y_{rot} (cm)	μ (deg.)	Δ_0 $D=1$ cm	Δ $D=3.0$ cm
0	0	45° 00'	1.000	3.000	0.35	1.071	20° 55'	1.321	3.963
0.01	0.029	44 12	1.013	3.039	0.36	1.105	20 19	1.326	3.978
0.02	0.057	43 24	1.028	3.084	0.37	1.141	19 42	1.331	3.993
0.03	0.086	42 37	1.041	3.123	0.38	1.177	19 06	1.336	4.008
0.04	0.115	41 51	1.053	3.159	0.39	1.213	18 29	1.341	4.023
0.05	0.143	41° 05'	1.066	3.198	0.40	1.250	17° 55'	1.346	4.038
0.06	0.172	40 20	1.078	3.234	0.41	1.288	17 17	1.350	4.050
0.07	0.201	39 35	1.090	3.270	0.42	1.326	16 41	1.355	4.065
0.08	0.230	38 50	1.102	3.306	0.43	1.365	16 06	1.359	4.077
0.09	0.259	38 06	1.113	3.339	0.44	1.404	15 30	1.363	4.089
0.10	0.288	37° 25'	1.123	3.369	0.45	1.444	14° 54'	1.367	4.101
0.11	0.317	36 40	1.134	3.402	0.46	1.484	14 19	1.370	4.110
0.12	0.346	35 57	1.145	3.435	0.47	1.525	13 43	1.374	4.122
0.13	0.376	35 15	1.155	3.465	0.48	1.568	13 08	1.377	4.131
0.14	0.405	34 33	1.165	3.495	0.49	1.610	12 33	1.380	4.140
0.15	0.435	33° 52'	1.174	3.522	0.50	1.654	11° 57'	1.384	4.152
0.16	0.464	33 10	1.184	3.552	0.51	1.699	11 22	1.386	4.158
0.17	0.494	32 29	1.193	3.579	0.52	1.744	10 47	1.389	4.167
0.18	0.524	31 49	1.202	3.606	0.53	1.791	10 12	1.392	4.176
0.19	0.554	31 08	1.211	3.633	0.54	1.838	9 37	1.394	4.182
0.20	0.585	30° 28'	1.219	3.657	0.55	1.887	9° 02'	1.397	4.191
0.21	0.615	29 49	1.227	3.681	0.56	1.937	8 28	1.399	4.197
0.22	0.646	29 09	1.235	3.705	0.57	1.988	7 53	1.401	4.203
0.23	0.677	28 30	1.243	3.729	0.58	2.040	7 18	1.403	4.209
0.24	0.708	27 51	1.250	3.750	0.59	2.094	6 44	1.404	4.212
0.25	0.740	27° 12'	1.258	3.774	0.60	2.149	6° 09'	1.406	4.218
0.26	0.771	26 34	1.265	3.795	0.61	2.206	5 34	1.408	4.224
0.27	0.803	25 55	1.272	3.816	0.62	2.264	5 00	1.409	4.227
0.28	0.836	25 17	1.279	3.837	0.63	2.324	4 25	1.410	4.230
0.29	0.868	24 39	1.285	3.855	0.64	2.386	3 51	1.411	4.233
0.30	0.901	24° 01'	1.292	3.876	0.65	2.451	3° 17'	1.412	4.236
0.31	0.934	23 24	1.298	3.894	0.66	2.517	2 42	1.413	4.239
0.32	0.968	22 47	1.304	3.912	0.67	2.586	2 08	1.413	4.239
0.33	1.002	22 09	1.310	3.930	0.68	2.657	1 33	1.414	4.242
0.34	1.036	21 32	1.315	3.945	0.69	2.731	0 59	1.414	4.242

4.6. Random-orientation Methods

The powder method has been fully described in various textbooks (References [1, 11, 12], etc.).

Many published tables are available for transforming from measured 2θ angles to interplanar spacings in Å. These are convenient, but the wavelength values used depend to a certain extent on an arbitrary selection of experimental data and of the still uncertain value of the $kX/\text{Å}$ conversion factor. (The information available will be brought up to date in Volume III.) They should only be used to give spacings in Å correct to three decimal places.

- [1] SWITZER, G., AXELROD, J. M., LINDBERG, M. L., and LARSEN, E. S., 3rd, *Tables of d Spacings for Angle 2θ ; $\text{CuK}\alpha$, $\text{CuK}\alpha_1$, $\text{CuK}\alpha_2$, $\text{FeK}\alpha$, $\text{FeK}\alpha_1$, $\text{FeK}\alpha_2$* . U.S. Geological Survey Circular 29 (1948). $2\theta=2\cdot0(0\cdot1)150\cdot9$ for $\text{K}\alpha$; $2\theta=90\cdot0(0\cdot1)175\cdot9$ for $\text{K}\alpha_1$ and $\text{K}\alpha_2$; 5 sign. figs.
- [2] *Tables for Conversion of X-ray Diffraction Angles in Interplanar Spacing*. U.S. National Bureau of Standards (1950). $\text{MoK}\alpha_1$, $\text{CuK}\alpha_1$, $\text{NiK}\alpha_1$, $\text{CoK}\alpha_1$, $\text{FeK}\alpha_1$, $\text{CrK}\alpha_1$, $\theta=0(0\cdot1)89\cdot99$; $\text{CuK}\alpha_1$, $\text{FeK}\alpha_1$, $2\theta=0(0\cdot02)179\cdot99$; 5 sign. figs.
- [3] PARRISH, W., and IRWIN, B. W. *Charts for the Solution of Bragg's Equation (d versus θ , 2θ)*. Philips Technical Library, Eindhoven (1953). Graphs of d vs. θ and 2θ graduated at intervals $0\cdot01^\circ$ in θ , for $\text{K}\alpha$, $\text{K}\alpha_1$, $\text{K}\alpha_2$, $\text{K}\beta$ lines of Cr, Fe, Cu and Mo.
- [4] BEATTY, SUZANNE. *Table of Interplanar Spacings in Angström Units in Terms of 2θ for Different Target Materials*. Westinghouse Research Laboratories, East Pittsburgh, Penna. (1948): Research Report R-94602-10-C, $\text{K}\alpha_1$ for Mo, Cu, Co, Fe and Cr, $2\theta=5\cdot0(0\cdot1)85\cdot0$, 4 sign. figs.; Research Report R-94602-10-E, same except $2\theta=85\cdot0(0\cdot1)176\cdot9$.

It is often convenient to make an estimate, with a ruler, of the 2θ values for certain lines and to convert these quickly to approximate d values. Comparison of angles for different wavelengths is also needed when, for example, a contaminating radiation is suspected of having introduced spurious lines into the powder pattern. Similar information is frequently useful in the study of single crystals. Table 4.6 is therefore included here as an aid in this approximate procedure.

4.6.1. Indexing Powder Patterns, given Lattice Constants

When the lattice constants of a crystal are known, either the $\sin^2 \theta$ or the d values to be expected may be compared with those of the observed powder diffraction lines and each line thus identified and indexed. The calculations of d are best carried out by evaluating the reciprocal components \bar{x} , \bar{y} , and \bar{z} for each (hkl) from the Cartesian matrix according to the relation†:

$$\begin{pmatrix} a_{11} & 0 & a_{13} \\ a_{21} & a_{22} & a_{23} \\ 0 & 0 & a_{33} \end{pmatrix} \times \begin{pmatrix} h \\ k \\ l \end{pmatrix} = (\bar{x}\bar{y}\bar{z})$$

Then

$$d_{hkl} = \frac{1}{\sqrt{(\bar{x})^2 + (\bar{y})^2 + (\bar{z})^2}}$$

The six non-zero elements of the Cartesian matrix depend on the lattice constants according to the scheme set out below:

† The actual coefficients of this matrix will depend on the orientation of the Cartesian axes \mathbf{a}' , \mathbf{b}' , \mathbf{c}' relative to the original axes \mathbf{a} , \mathbf{b} , \mathbf{c} . The matrix given here corresponds to \mathbf{b}' coincident with \mathbf{b} , \mathbf{a}' in the obtuse γ angle in the ab plane and \mathbf{c}' perpendicular to \mathbf{a}' and \mathbf{b}' (and hence coincident with the reciprocal axis \mathbf{c}^*). In Section 2 another convention is adopted. There is no standard convention, and therefore care must be taken to observe consistency.

System	a_{11}	a_{13}	a_{21}	a_{22}	a_{23}	a_{33}
Cubic	$\frac{1}{a_0}$	0	0	$\frac{1}{a_0}$	0	$\frac{1}{a_0}$
Hexagonal	$\frac{1}{a_0}$	0	$\frac{1}{(\sqrt{3})a_0}$	$\frac{2}{(\sqrt{3})a_0}$	0	$\frac{1}{c_0}$
Tetragonal	$\frac{1}{a_0}$	0	0	$\frac{1}{a_0}$	0	$\frac{1}{c_0}$
Orthorhombic	$\frac{1}{a_0}$	0	0	$\frac{1}{b_0}$	0	$\frac{1}{c_0}$
Monoclinic	$\frac{1}{a_0 \sin \beta}$	$-\frac{\cot \beta}{c_0}$	0	$\frac{1}{b_0}$	0	$\frac{1}{c_0}$
Triclinic	$\frac{1}{a_0 \sin \beta}$	$-\frac{\cot \beta}{c_0}$	$-\frac{v_1}{a_0 v_2 \sin \beta}$	$\frac{1}{b_0 v_2}$	$\frac{v_1 \cot \beta - \cos \alpha}{c_0 v_2}$	$\frac{1}{c_0}$

where

$$v_1 = \frac{\cos \gamma - \cos \alpha \cos \beta}{\sin \beta}$$

$$v_2 = \frac{\sqrt{(1 + 2 \cos \alpha \cos \beta \cos \gamma - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma)}}{\sin \beta}$$

The tables given in Section 3 (3.5.6, 3.6.6, 3.8.6A) for h^2+k^2 , h^2+k^2+hk , $h^2+k^2+l^2$ may also be used for high-symmetry structures.

4.6.2. Determining Unknown Lattice Constants

Cubic patterns are distinguished by the fact that all reciprocal spacings are equal to a constant (the reciprocal unit-cell axis) multiplied by the square root of an integer which is the sum of three squares:

$$\frac{1}{d} = \frac{\sqrt{(h^2+k^2+l^2)}}{a} \quad \dots (1)$$

The values of hkl and of a are therefore easily found.

All methods of determining hkl and the lattice constants for structures of lower symmetry depend on some sort of trial-and-error routine. The problem can be solved in general for tetragonal and hexagonal crystals because only one variable parameter need be

determined. The method has been applied in Section 4.3.4 to the indexing of the zero-layer line corresponding to an orthogonal ($hk0$) net. It is now extended to the three-dimensional case. C. W. Bunn ([5]; but see footnote to 4.3.4, p. 184) writes the formula for d in a form equivalent to the following:

$$\log \left(\frac{1}{d^2} \right) = \log [p + (r-1)l^2] + \log \left(\frac{q}{a^2} \right) \quad \dots (2)$$

$$\left. \begin{array}{l} p = h^2 + k^2 \\ q = 1 \end{array} \right\} \text{for tetragonal}$$

$$\left. \begin{array}{l} p = h^2 + k^2 + hk \\ q = 4/3 \end{array} \right\} \text{for hexagonal}$$

$$r = \frac{1 + q(c/a)^2}{q(c/a)^2}$$

Tables 4.6.2A and B give data for the construction of charts of the type of Figs. 4.6.2(1) and (2). These represent the variation of $2 \log (1/d)$ with c/a for all (hkl) within the given range. Any useful function of c/a may be used for the abscissae (compare, for instance, Fig. 4.3.4, which was drawn with a linear scale of b/a). The method of using the chart has already been described in Section 4.3.4.

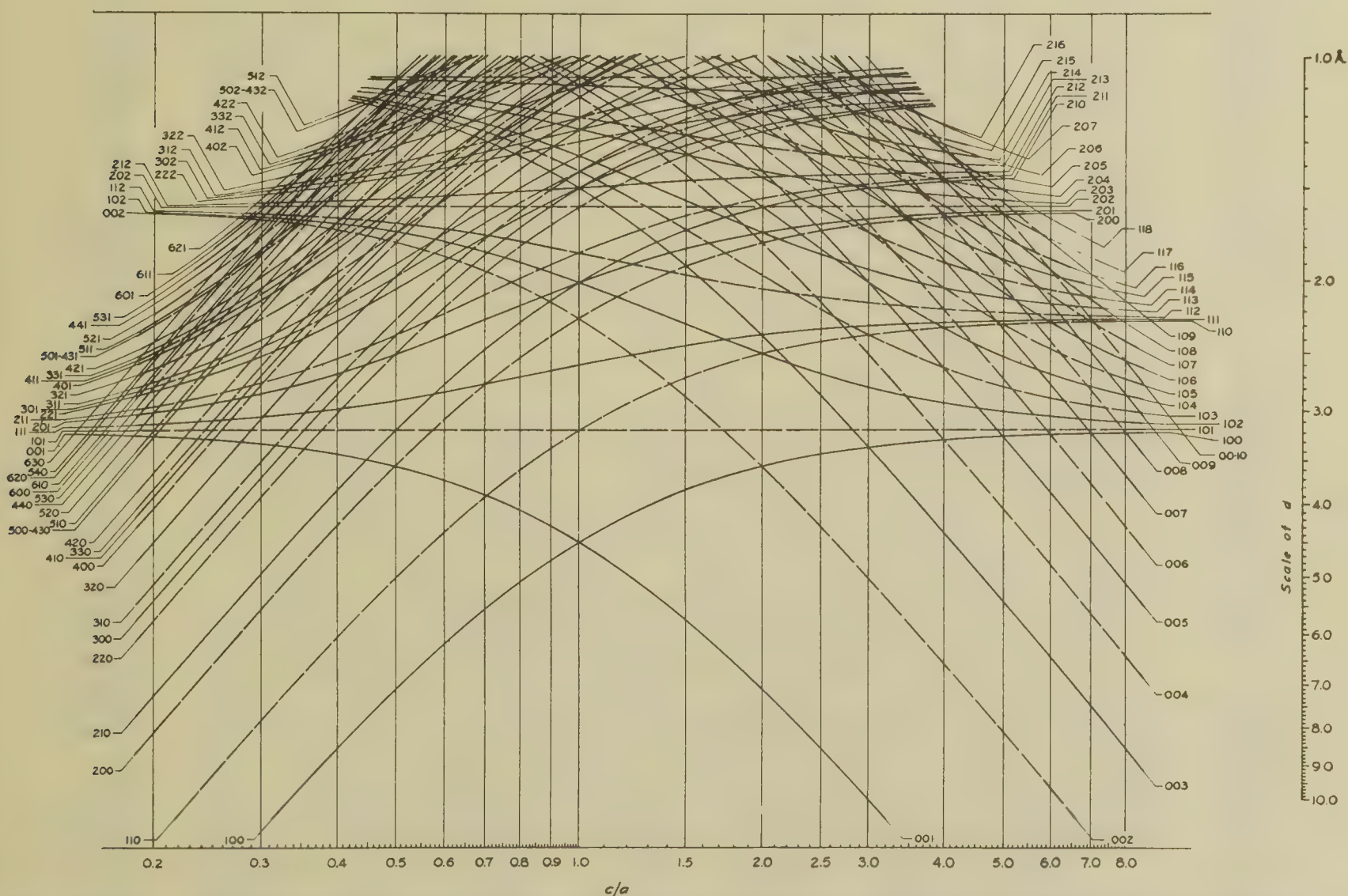


Fig. 4.6.2(1). Layout of Bunn chart for indexing tetragonal powder photographs; dashed lines correspond to body-centred lattice. To be effective, this chart must be drawn to very large scale.

4.6. RANDOM-ORIENTATION METHODS

TABLE 4.6

Quick-reference Table of d (Spacings) vs. Bragg Angle for Various Mean Wavelengths

$\lambda, \text{\AA}$	CrK α 2.290(9)	FeK α 1.937(3)	CoK α 1.790(2)	NiK α 1.659(1)	CuK α 1.541(8)	MoK α 0.710(7)	RhK α 0.614(7)	AgK α 0.560(9)
2θ								
0	∞							
1	131.3	111.0	102.6	95.1	88.3	40.7(2)	35.2(2)	32.1(4)
2	65.6(3)	55.5(0)	51.2(9)	47.5(3)	44.1(7)	20.3(6)	17.6(1)	16.0(7)
3	43.7(6)	37.0(0)	34.1(9)	31.6(9)	29.4(5)	13.5(7)	11.6(9)	10.7(1)
4	32.8(2)	27.7(6)	25.6(5)	23.7(7)	22.0(9)	10.1(8)	8.81	8.04
5	26.26	22.21	20.52	19.02	17.67	8.15	7.05	6.43
6	21.89	18.51	17.10	15.85	14.73	6.79	5.87	5.36
7	18.76	15.87	14.66	13.59	12.63	5.82	5.03	4.59
8	16.42	13.89	12.83	11.89	11.05	5.09	4.41	4.02
9	14.60	12.35	11.41	10.57	9.83	4.53	3.92	3.57
10	13.14	11.11	10.27	9.52	8.85	4.08	3.53	3.22
11	11.95	10.11	9.34	8.65	8.04	3.71	3.21	2.93
12	10.96	9.27	8.56	7.94	7.38	3.40	2.94	2.68
13	10.12	8.56	7.91	7.33	6.81	3.14	2.72	2.48
14	9.40	7.95	7.34	6.81	6.33	2.92	2.52	2.30
15	8.78	7.42	6.86	6.36	5.91	2.72	2.355	2.148
16	8.23	6.96	6.43	5.96	5.54	2.55	2.208	2.015
17	7.75	6.55	6.06	5.61	5.22	2.40	2.079	1.897
18	7.32	6.19	5.72	5.30	4.93	2.27	1.965	1.793
19	6.94	5.87	5.42	5.03	4.67	2.15	1.862	1.699
20	6.60	5.58	5.15	4.78	4.44	2.046	1.770	1.615
21	6.29	5.32	4.91	4.55	4.23	1.950	1.687	1.539
22	6.01	5.08	4.69	4.35	4.04	1.862	1.611	1.470
23	5.75	4.86	4.49	4.16	3.87	1.782	1.542	1.407
24	5.51	4.66	4.31	3.99	3.71	1.709	1.478	1.349
25	5.29	4.48	4.14	3.833	3.562	1.642	1.420	1.296
26	5.09	4.31	3.98	3.688	3.427	1.580	1.366	1.247
27	4.91	4.15	3.83	3.553	3.302	1.522	1.316	1.201
28	4.73	4.00	3.70	3.429	3.187	1.469	1.270	1.159
29	4.57	3.87	3.58	3.313	3.079	1.419	1.228	1.120
30	4.43	3.743	3.458	3.205	2.979	1.373	1.188	1.084
31	4.29	3.625	3.349	3.104	2.885	1.330	1.150	1.049
32	4.16	3.514	3.247	3.009	2.797	1.289	1.115	1.017
33	4.03	3.411	3.152	2.921	2.714	1.251	1.082	0.987
34	3.92	3.313	3.062	2.837	2.637	1.215	1.051	0.959
35	3.809	3.221	2.977	2.759	2.564	1.182	1.022	0.933
36	3.707	3.135	2.897	2.684	2.495	1.150	0.995	0.908
37	3.610	3.053	2.821	2.614	2.430	1.120	0.969	0.884
38	3.518	2.975	2.749	2.548	2.368	1.091	0.944	0.861
39	3.431	2.902	2.681	2.485	2.309	1.065	0.921	0.840

4.6. RANDOM-ORIENTATION METHODS

TABLE 4.6 (*continued*)

λ , Å	CrK α 2.290(9)	FeK α 1.937(3)	CoK α 1.790(2)	NiK α 1.659(1)	CuK α 1.541(8)	MoK α 0.710(7)	RhK α 0.614(7)	AgK α 0.560(9)
2 θ								
40	3.349	2.832	2.617	2.425	2.254	1.039	0.899	0.820
41	3.271	2.766	2.556	2.369	2.201	1.015	0.878	0.801
42	3.196	2.703	2.498	2.315	2.151	0.992	0.858	0.783
43	3.125	2.643	2.442	2.263	2.103	0.970	0.839	0.766
44	3.058	2.586	2.389	2.214	2.058	0.949	0.820	0.749
45	2.993	2.531	2.339	2.168	2.014	0.929	0.803	0.733
46	2.931	2.479	2.291	2.123	1.973	0.909	0.787	0.718
47	2.873	2.429	2.245	2.080	1.933	0.891	0.771	0.703
48	2.817	2.381	2.201	2.040	1.895	0.874	0.756	0.689
49	2.762	2.336	2.158	2.001	1.859	0.857	0.741	0.676
50	2.710	2.292	2.118	1.963	1.824	0.841	0.727	0.663
51	2.661	2.250	2.079	1.927	1.791	0.825	0.714	0.651
52	2.613	2.210	2.042	1.892	1.759	0.810	0.701	0.640
53	2.567	2.171	2.006	1.859	1.728	0.796	0.689	0.629
54	2.523	2.134	1.972	1.827	1.698	0.783	0.677	0.618
55	2.481	2.098	1.939	1.797	1.669	0.770	0.666	0.607
56	2.440	2.063	1.907	1.767	1.642	0.757	0.655	0.597
57	2.401	2.030	1.876	1.739	1.616	0.745	0.644	0.587
58	2.363	1.998	1.846	1.711	1.590	0.733	0.634	0.578
59	2.326	1.967	1.818	1.685	1.566	0.722	0.624	0.569
60	2.291	1.937	1.791	1.659	1.542	0.711	0.615	0.561
61	2.257	1.909	1.764	1.634	1.519	0.700	0.606	0.553
62	2.224	1.881	1.738	1.611	1.497	0.690	0.597	0.545
63	2.192	1.854	1.713	1.588	1.476	0.680	0.588	0.537
64	2.162	1.828	1.689	1.565	1.455	0.670	0.580	0.529
65	2.132	1.803	1.666	1.544	1.435	0.661	0.572	0.522
66	2.103	1.779	1.644	1.523	1.415	0.652	0.564	0.515
67	2.075	1.755	1.622	1.503	1.397	0.643	0.557	0.508
68	2.048	1.732	1.601	1.483	1.379	0.635	0.550	0.502
69	2.022	1.712	1.581	1.464	1.361	0.627	0.543	0.496
70	1.997	1.689	1.561	1.446	1.344	0.620	0.536	0.489
71	1.973	1.668	1.542	1.429	1.328	0.612	0.529	0.483
72	1.949	1.648	1.523	1.412	1.312	0.604	0.523	0.477
73	1.926	1.628	1.505	1.395	1.296	0.597	0.517	0.471
74	1.903	1.610	1.487	1.378	1.281	0.590	0.511	0.466
75	1.882	1.591	1.470	1.362	1.266	0.584	0.505	0.461
76	1.861	1.573	1.454	1.347	1.252	0.577	0.499	0.456
77	1.840	1.556	1.438	1.332	1.238	0.571	0.494	0.451
78	1.820	1.539	1.422	1.318	1.225	0.565	0.488	0.446
79	1.801	1.523	1.407	1.304	1.212	0.559	0.483	0.441
80	1.782	1.507	1.393	1.291	1.200	0.553	0.478	0.436

4.6. RANDOM-ORIENTATION METHODS

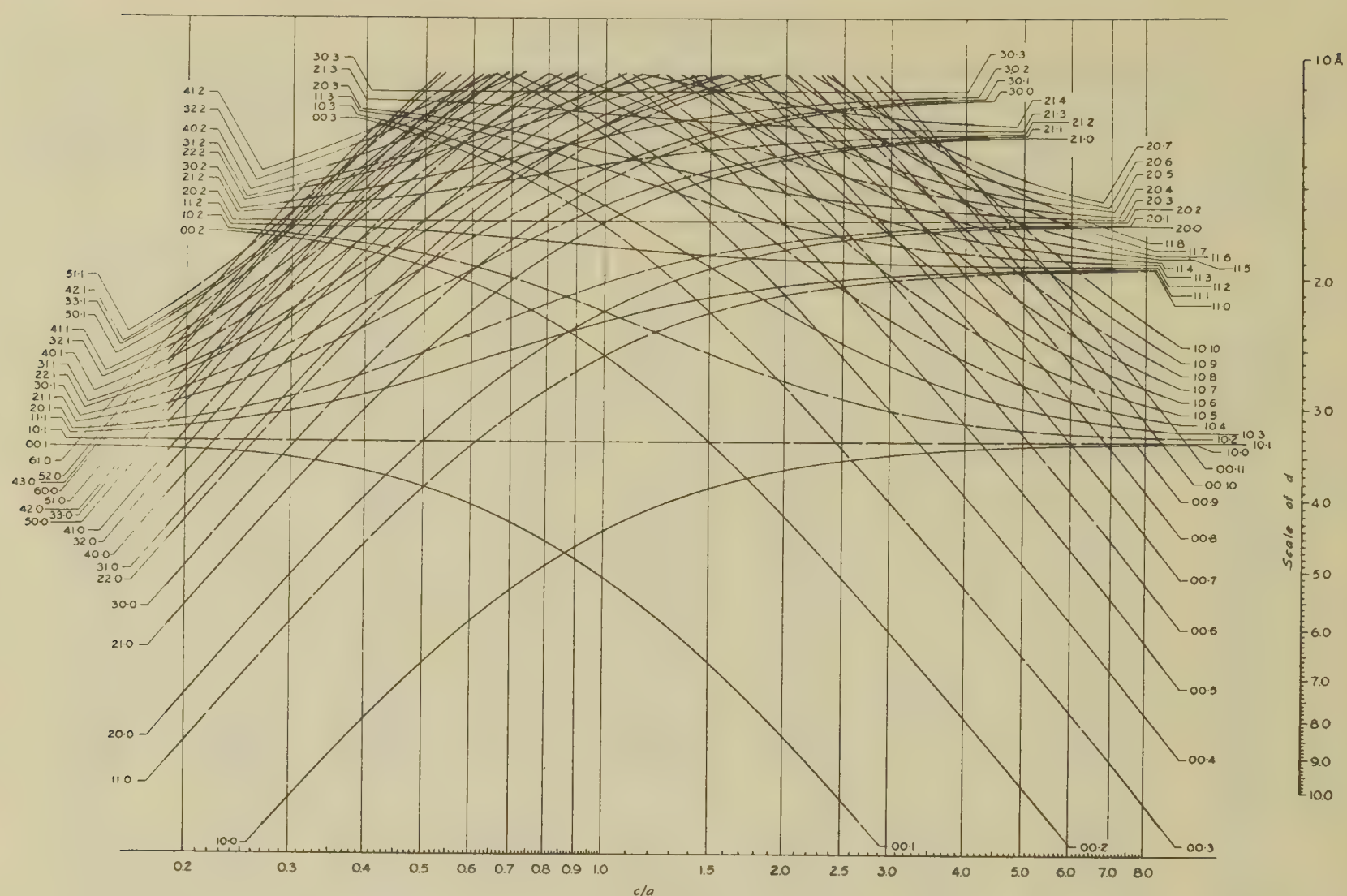


Fig. 4.6.2(2). Layout of Bunn chart for indexing hexagonal powder photographs; dashed lines correspond to rhombohedral lattice. To be effective, this chart must be drawn to very large scale.

No entirely satisfactory method exists for interpreting powder diagrams for systems of lower symmetry. A general method devised by Ito [42] is as follows.

The formula for d in terms of the reciprocal-lattice constants is

$$\frac{1}{d^2} = \Sigma h^2 a^{*2} + 2 \Sigma k l b^* c^* \cos \alpha^*$$

Let any triplet of lines be taken as corresponding to first-order reflections 100, 010, 001. (In practice one would probably take the first three lines of largest spacing.) These fix a^* , b^* , c^* , since $1/d_{100} = a^*$, etc.

Suppose $\beta^* = 90^\circ$. Then the 101 and $10\bar{1}$ reflections would occur with a spacing given by

$$\frac{1}{d_{101}^2} = a^{*2} + c^{*2}$$

If, however, $\beta^* \neq 90^\circ$, the actual spacings will be

$$\frac{1}{d_{101}^2} = a^{*2} + c^{*2} + 2a^*c^* \cos \beta^*$$

$$\frac{1}{d_{10\bar{1}}^2} = a^{*2} + c^{*2} - 2a^*c^* \cos \beta^*$$

The $1/d^2$ values of the 101, $10\bar{1}$ reflections will be symmetrical with respect to the hypothetical ($\beta^* = 90^\circ$)

value first calculated; and if they actually occur on the photograph they can be recognized by this symmetry and will allow the determination of the β^* angle as follows:

$$\cos \beta^* = \frac{1/d_{101}^2 - 1/d_{10\bar{1}}^2}{4a^*c^*}$$

Any pair of $h0l$, $h0\bar{l}$ can be similarly used.

$$\cos \beta^* = \frac{1/d_{h0l}^2 - 1/d_{h0\bar{l}}^2}{4hla^*c^*}$$

If no suitable pair is available, a different triplet of reflections must be chosen as the axial reflections 100, 010, 001 or as the higher orders of these reflections. Hence also α^* and γ^* .

A survey of observed and calculated $1/d^2$ values will show whether the constants of the reciprocal lattice have been correctly determined and whether the corresponding direct lattice is a Bravais lattice or is a more primitive or more complex lattice. This method can be applied also to random-rotation photographs, but it depends for its application on the accuracy of the measured data and it is not easily applied when there are systematic space-group absences. Reference should be made to the original papers, and also to [41] [43] [44] [45].

4.6. RANDOM-ORIENTATION METHODS

TABLE 4.6.2A

Data for Construction of Bunn Chart for indexing Tetragonal Powder Patterns

Tabulated values are $2 \log (1/d) + \text{constant}$

I denotes a reflection in a body-centred lattice

Scale of chart should allow 1.0 table unit = 30 cm or more

c/a	$\log (c/a)$	001	002 I	003	004 I	005	006 I	007
0.2	-0.6990	0.9830						
0.3	-0.5229	0.9626	1.5646					
0.4	-0.3979	0.9355	1.5376					
0.5	-0.3010	0.9031	1.5052	1.8573				
0.6	-0.2218	0.8665	1.4685	1.8203				
0.8	-0.0969	0.7852	1.3872	1.7394				
1.0	0	0.6990	1.3010	1.6532	1.9031			
1.5	0.1761	0.4881	1.0902	1.4424	1.6922	1.8861		
2.0	0.3010	0.3010	0.9031	1.2553	1.5052	1.6990	1.8573	
2.5	0.3979	0.1397	0.7417	1.0939	1.3438	1.5376	1.6960	1.8299
3.0	0.4771	0	0.6021	0.9542	1.2041	1.3979	1.5563	1.6902
4.0	0.6021	-0.2305	0.3716	0.7238	0.9737	1.1675	1.3258	1.4597
5.0	0.6990		0.1871	0.5393	0.7891	0.9830	1.1413	1.2752
6.0	0.7782		0.0338	0.3860	0.6360	0.8298	0.9881	1.1220
8.0	0.9031		-0.2110	0.1412	0.3911	0.5849	0.7432	0.8772

c/a	008 I	009	0010 I	100	101 I	102	103 I	104
0.2					1.0000			
0.3				-0.0832	1.0000			
0.4				0.1397	1.0000	1.5546		
0.5				0.3010	1.0000	1.5315	1.8692	
0.6				0.4228	1.0000	1.5059	1.8377	
0.8				0.5931	1.0000	1.4517	1.7692	
1.0				0.6990	1.0000	1.3979	1.6990	1.9294
1.5				0.8403	1.0000	1.2840	1.5393	1.7494
2.0				0.9031	1.0000	1.2041	1.4150	1.6031
2.5	1.9458			0.9355	1.0000	1.1504	1.3229	1.4870
3.0	1.8062	1.9085		0.9542	1.0000	1.1139	1.2553	1.3979
4.0	1.5757	1.6780	1.7695	0.9737	1.0000	1.0706	1.1674	1.2747
5.0	1.3912	1.4935	1.5849	0.9830	1.0000	1.0474	1.1165	1.1978
6.0	1.2381	1.3403	1.4319	0.9881	1.0000	1.0338	1.0850	1.1478
8.0	0.9932	1.0954	1.1870	0.9933	1.0000	1.0195	1.0504	1.0901

4.6. RANDOM-ORIENTATION METHODS

TABLE 4.6.2A (*continued*)

Data for Construction of Bunn Chart for indexing Tetragonal Powder Patterns

Tabulated values are $2 \log (1/d) + \text{constant}$

I denotes a reflection in a body-centred lattice

Scale of chart should allow 1.0 table unit = 30 cm or more

c/a	105 I	106	107 I	108	109 I
1.5	1.9235				
2.0	1.7634	1.9031			
2.5	1.6345	1.7655	1.8820		
3.0	1.5315	1.6532	1.7634	1.8633	1.9542
4.0	1.3823	1.4855	1.5824	1.6726	1.7563
5.0	1.2840	1.3703	1.4542	1.5344	1.6103
6.0	1.2171	1.2892	1.3612	1.4319	
8.0	1.1364	1.1870			

c/a	110 I	111	112 I	113	114 I	115	116 I	117	118 I
0.2	-0.1139	1.0164							
0.3	0.2178	1.0344							
0.4	0.4407	1.0561	1.5710						
0.5	0.6021	1.0792	1.5563	1.8808					
0.6	0.7238	1.1020	1.5404	1.8541					
0.8	0.8923	1.1430	1.5078	1.7972					
1.0	1.0000	1.1761	1.4771	1.7404	1.9542				
1.5	1.1413	1.2285	1.4175	1.6184	1.7999				
2.0	1.2041	1.2553	1.3802	1.5315	1.6812	1.8195	1.9445		
2.5	1.2366	1.2700	1.3571	1.4721	1.5942	1.7137	1.8254	1.9285	
3.0	1.2553	1.2788	1.3424	1.4314	1.5315	1.6335	1.7324	1.8261	1.9138
4.0	1.2747	1.2881	1.3258	1.3823	1.4508	1.5254	1.6020	1.6780	1.7518
5.0	1.2838	1.2926	1.3174	1.3558	1.4045	1.4601	1.5195	1.5806	
6.0	1.2891	1.2951	1.3126	1.3403	1.3763	1.4186			

4.6. RANDOM-ORIENTATION METHODS

TABLE 4.6.2A (*continued*)

Data for Construction of Bunn Chart for indexing Tetragonal Powder Patterns

Tabulated values are $2 \log (1/d) + \text{constant}$

I denotes a reflection in a body-centred lattice

Scale of chart should allow 1.0 table unit = 30 cm or more

c/a	200 I	201	202 I	203	204 I	205	206 I	207
0.2	0.1871	1.0474						
0.3	0.5189	1.0961						
0.4	0.7417	1.1504	1.6021					
0.5	0.9031	1.2041	1.6021	1.9031				
0.6	1.0292	1.2538	1.6021	1.8852				
0.8	1.1934	1.3366	1.6021	1.8481				
1.0	1.3010	1.3979	1.6021	1.8129				
1.5	1.4423	1.4881	1.6021	1.7434	1.8821			
2.0	1.5052	1.5315	1.6021	1.6990	1.8062	1.9138		
2.5	1.5376	1.5546	1.6021	1.6711	1.7524	1.8386	1.9250	
3.0	1.5563	1.5682	1.6021	1.6532	1.7160	1.7853	1.8573	1.9294
4.0	1.5757	1.5825	1.6021	1.6329	1.6745	1.7189		

c/a	210	211 I	212	213 I	214	215 I	216
0.2	0.2840	1.0621					
0.3	0.6158	1.1240					
0.4	0.8386	1.1908	1.6167				
0.5	1.0000	1.2553	1.6233	1.9138			
0.6	1.1217	1.3136	1.6299	1.8999			
0.8	1.2903	1.4084	1.6425	1.8715			
1.0	1.3979	1.4771	1.6532	1.8451			
1.5	1.5393	1.5763	1.6714	1.7945	1.9235		
2.0	1.6021	1.6233	1.6812	1.7634	1.8573	1.9542	
2.5	1.6348	1.6482	1.6868	1.7417	1.8141	1.8898	
3.0	1.6532	1.6628	1.6902	1.7324	1.7853	1.8451	1.9085
4.0	1.6726	1.6780	1.6939	1.7190	1.7518		

4.6. RANDOM-ORIENTATION METHODS

TABLE 4.6.2A (*continued*)
Data for Construction of Bunn Chart for indexing Tetragonal Powder Patterns

Tabulated values are $2 \log (1/d) + \text{constant}$
 I denotes a reflection in a body-centred lattice
 Scale of chart should allow 1.0 table unit = 30 cm or more

c/a	220 I	221	222 I	223	300	301 I	302	303 I
0.2	0.4881	1.1035			0.5393	1.1165		
0.3	0.8199	1.1980			0.8711	1.2203		
0.4	1.0428	1.2934	1.6582		1.0939	1.3229	1.6711	
0.5	1.2041	1.3802	1.6812	1.9445	1.2553	1.4150	1.6990	1.9542
0.6	1.3259	1.4553	1.7040	1.9413	1.3770	1.4938	1.7262	1.9542
0.8	1.4944	1.5719	1.7451	1.9350	1.5456	1.6151	1.7746	1.9542
1.0	1.6021	1.6532	1.7782	1.9294	1.6532	1.6990	1.8129	1.9542
1.5	1.7434	1.7669	1.8305	1.9195	1.7945	1.8155	1.8728	1.9542
2.0	1.8062	1.8195	1.8573	1.9138	1.8573	1.8692	1.9031	1.9542
2.5	1.8386	1.8472	1.8721	1.9105	1.8898	1.8974	1.9196	1.9542
3.0	1.8573	1.8633	1.8808	1.9085	1.9085	1.9138	1.9294	1.9542

c/a	310 I	320	400 I	410	330 I	420 I	500-430	510 I
0.2	0.5850	0.6990	0.7891	0.8155	0.8403	0.8860	0.9830	1.0000
0.3	0.9168	1.0308	1.1209	1.1462	1.1721	1.2178	1.3148	1.3318
0.4	1.1397	1.2537	1.3439	1.3701	1.3949	1.4407	1.5432	1.5517
0.5	1.3010	1.4150	1.5052	1.5315	1.5563	1.6021	1.6990	1.7160
0.6	1.4228	1.5411	1.6269	1.6532	1.6780	1.7238	1.8207	1.8378
0.8	1.5913	1.7053	1.6954	1.8218	1.8466	1.8924		
1.0	1.6990	1.8129	1.9031	1.9294	1.9542			
1.5	1.8403	1.9542						
2.0	1.9031							
2.5	1.9355							
3.0	1.9542							

c/a	520	440 I	530 I	600 I	610	620 I	540	630
0.2	1.0474	1.0902	1.1165	1.1413	1.1532	1.1871	1.1978	1.2382
0.3	1.3792	1.4219	1.4483	1.4731	1.4850	1.5189	1.5296	1.5700
0.4	1.6021	1.6448	1.6711	1.6960	1.7079	1.7417	1.7525	1.7929
0.5	1.7634	1.8062	1.8325	1.8573	1.8692	1.9031	1.9138	1.9542
0.6	1.8852	1.9279	1.9543					

4.6. RANDOM-ORIENTATION METHODS

TABLE 4.6.2A (continued)

Data for Construction of Bunn Chart for indexing Tetragonal Powder Patterns

Tabulated values are $2 \log (1/d) + \text{constant}$

I denotes a reflection in a body-centred lattice

Scale of chart should allow 1.0 table unit = 30 cm or more

c/a	311	321 I	401	411 I	331	421	501-431 I	511
0.2	1.1291	1.1648	1.1978	1.2082	1.2185	1.2499		
0.3	1.2413	1.2991	1.3499	1.3657	1.3808	1.4098	1.4744	1.4863
0.4	1.3505	1.4241	1.4870	1.5061	1.5244	1.5588	1.6345	1.6481
0.5	1.4472	1.5315	1.6021	1.6233	1.6435	1.6812	1.7634	1.7782
0.6	1.5292	1.6208	1.6964	1.7189	1.7404	1.7803	1.8665	1.8818
0.8	1.6544	1.7546	1.8359	1.8600	1.8828	1.9250		
1.0	1.7404	1.8451	1.9294	1.9542				
1.5	1.8592							
2.0	1.9138							
2.5	1.9424							

c/a	521 I	441	531	601	611 I	621
0.3	1.5200	1.5514				
0.4	1.6868	1.7223	1.7417	1.7655	1.7756	
0.5	1.8195	1.8573	1.8808	1.9031	1.9138	1.9445
0.6	1.9249					

c/a	312 I	322	402 I	412	332 I	422 I	502-432	512 I
0.4	1.6837	1.7194	1.7524	1.7629	1.7731	1.7929		
0.5	1.7160	1.7634	1.8062	1.8295	1.8325	1.8573	1.9138	1.9243
0.6	1.7473	1.8050	1.8559	1.8716	1.8868	1.9157		
0.8	1.8022	1.8758	1.9387					
1.0	1.8451	1.9294						
1.5	1.9114							
2.0	1.9445							

TABLE 4.6.2B

Data for Construction of Bunn Chart for indexing Hexagonal Powder Patterns

Tabulated values are $2 \log (1/d) + \text{constant}$ R denotes a reflection in a rhombohedral lattice ($-h+k+l=3n$)

Scale of chart should allow 1.0 table unit = 30 cm or more

c/a	$\log (c/a)$	00·1	00·2	00·3 R	00·4	00·5	00·6 R	00·7
0·2	-0·6990	0·9774						
0·3	-0·5229	0·9508	1·5528					
0·4	-0·3979	0·9160	1·5181					
0·5	-0·3010	0·8751	1·4771	1·8293				
0·6	-0·2218	0·8297	1·4318	1·7840				
0·8	-0·0969	0·7320	1·3341	1·6863	1·9362			
1·0	0	0·6320	1·2341	1·5863	1·8361			
1·5	0·1761	0·3979	1·0000	1·3522	1·6021	1·7959	1·9542	
2·0	0·3010	0·1984	0·8004	1·1526	1·4023	1·5963	1·7547	1·8885
2·5	0·3979	0·0299	0·6320	0·9842	1·2341	1·4279	1·5863	1·7202
3·0	0·4771	-0·1140	0·4881	0·8403	1·0901	1·2840	1·4423	1·5762
4·0	0·6021		0·2531	0·6052	0·8551	1·0489	1·2073	1·3412
5·0	0·6990		0·0663	0·4185	0·6684	0·8622	1·0206	1·1545
6·0	0·7782		-0·0882	0·2640	0·5139	0·7077	0·8660	0·9999
8·0	0·9031			0·0178	0·2676	0·4614	0·6198	0·7537

c/a	00·8	00·9 R	00·10	00·11	10·0	10·1 R	10·2 R(01·2)	10·3
0·2					-0·2956	1·0000		
0·3					0·0299	1·0000	1·5657	
0·4					0·2450	1·0000	1·5406	
0·5					0·3979	1·0000	1·5119	1·8451
0·6					0·5110	1·0000	1·4810	1·8065
0·8					0·6632	1·0000	1·4181	1·7256
1·0					0·7570	1·0000	1·3591	1·6463
1·5					0·8751	1·0000	1·2430	1·4771
2·0					0·9254	1·0000	1·1684	1·3547
2·5	1·8361	1·9384			0·9508	1·0000	1·1211	1·2688
3·0	1·6922	1·7945	1·8861		0·9652	1·0000	1·0902	1·2083
4·0	1·4572	1·5595	1·6510	1·7381	0·9801	1·0000	1·0547	1·1390
5·0	1·2705	1·3727	1·4643	1·5471	0·9872	1·0000	1·0364	1·0910
6·0	1·1159	1·2182	1·3097	1·3925	0·9911	1·0000	1·0258	1·0657
8·0	0·8697	0·9720	1·0635	1·1463	0·9950	1·0000	1·0148	1·0384

4.6. RANDOM-ORIENTATION METHODS

TABLE 4.6.2B (continued)

Data for Construction of Bunn Chart for indexing Hexagonal Powder Patterns

Tabulated values are $2 \log (1/d) + \text{constant}$ R denotes a reflection in a rhombohedral lattice ($-h+k+l=3n$)

Scale of chart should allow 1.0 table unit = 30 cm or more

c/a	10.4 R	10.5 R(01.5)	10.6	10.7 R	10.8 R(01.8)	10.9	10.10 R	11.8
0.8	1.9587							
1.0	1.8709							
1.5	1.6767	1.8451						
2.0	1.5274	1.6803	1.8147	1.9334				
2.5	1.4162	1.5528	1.6767	1.7883	1.8893			
3.0	1.3332	1.4542	1.5673	1.6714	1.7669	1.8545	1.9353	1.8861
4.0	1.2231	1.3169	1.4094	1.4982	1.5821	1.6610	1.7350	1.7582
5.0	1.1574	1.2302	1.3052	1.3799	1.4525	1.5224	1.5892	
6.0	1.1160	1.1730	1.2340	1.2966	1.3590	1.4203	1.4800	
8.0	1.0695	1.1064	1.1477	1.1918	1.2380			

c/a	11.0 R	11.1	11.2	11.3 R	11.4	11.5	11.6 R	11.7
0.2	0.1816	1.0419						
0.3	0.5071	1.0843	1.5903					
0.4	0.7222	1.1309	1.5825					
0.5	0.8751	1.1761	1.5740	1.8751				
0.6	0.9881	1.2171	1.5654	1.8485				
0.8	1.1403	1.2835	1.5489	1.7950				
1.0	1.2341	1.3310	1.5351	1.7460	1.9331			
1.5	1.3522	1.3979	1.5119	1.6532	1.7959	1.9294		
2.0	1.4025	1.4288	1.4995	1.5963	1.7035	1.8111	1.9144	
2.5	1.4279	1.4449	1.4923	1.5614	1.6427	1.7289	1.8153	1.8992
3.0	1.4423	1.4542	1.4881	1.5393	1.6021	1.6714	1.7434	1.8155
4.0	1.4772	1.4640	1.4836	1.5143	1.5542	1.6004	1.6510	1.7041
5.0	1.4643	1.4686	1.4813	1.5017	1.5287	1.5612	1.5978	1.6375
6.0	1.4682	1.4712	1.4800	1.4945				

4.6. RANDOM-ORIENTATION METHODS

TABLE 4.6.2B (continued)

Data for Construction of Bunn Chart for indexing Hexagonal Powder Patterns

Tabulated values are $2 \log (1/d) + \text{constant}$ R denotes a reflection in a rhombohedral lattice ($-h+k+l=3n$)

Scale of chart should allow 1.0 table unit = 30 cm or more

c/a	20.0	20.1 R(02.1)	20.2 R	20.3	20.4 R(02.4)	20.5 R	20.6	20.7 R(02.7)
0.2	0.3065	1.0614						
0.3	0.6319	1.1211	1.6021					
0.4	0.8471	1.1840	1.6021					
0.5	1.0000	1.2430	1.6021	1.8893				
0.6	1.1130	1.2951	1.6021	1.8680				
0.8	1.2652	1.3768	1.6021	1.8259				
1.0	1.3590	1.4337	1.6021	1.7884				
1.5	1.4771	1.5119	1.6021	1.7202	1.8451			
2.0	1.5274	1.5473	1.6021	1.6803	1.7704	1.8642		
2.5	1.5528	1.5657	1.6021	1.6566	1.7231	1.7959	1.8709	
3.0	1.5623	1.5763	1.6021	1.6419	1.6922	1.7494	1.8103	1.8780
4.0	1.5822	1.5872	1.6021	1.6257	1.6568	1.6937	1.7350	1.7792
5.0	1.5892	1.5925	1.6021	1.6176	1.6384			

c/a	21.0	21.1 R	21.2 R(12.2)	21.3	21.4 R	30.0 R	30.1	30.2
0.2	0.5495	1.1152				0.6587	1.1477	
0.3	0.8751	1.2156	1.6356			0.9842	1.2688	
0.4	1.0902	1.3128	1.6559			1.1993	1.3814	1.6886
0.5	1.2430	1.3979	1.6767	1.9294		1.3522	1.4771	1.7202
0.6	1.3561	1.4692	1.6966	1.9218		1.4652	1.5556	1.7499
0.8	1.5083	1.5755	1.7309	1.9074		1.6174	1.6706	1.7995
1.0	1.6021	1.6463	1.7569	1.8953		1.7112	1.7460	1.8362
1.5	1.7202	1.7404	1.7959	1.8751	1.9661	1.8293	1.8451	1.8893
2.0	1.7705	1.7819	1.8147	1.8642	1.9254	1.8796	1.8885	1.9144
2.5	1.7959	1.8033	1.8247	1.8582	1.9011	1.9050	1.9107	1.9276
3.0	1.8103	1.8221	1.8305	1.8545	1.8861	1.9195	1.9235	1.9353
4.0	1.8252	1.8281	1.8367	1.8506	1.8694			

4.6. RANDOM-ORIENTATION METHODS

TABLE 4.6.2B (continued)

Data for Construction of Bunn Chart for indexing Hexagonal Powder Patterns

Tabulated values are $2 \log (1/d) + \text{constant}$ R denotes a reflection in a rhombohedral lattice ($-h+k+l=3n$)

Scale of chart should allow 1.0 table unit = 30 cm or more

c/a	30.0 R	22.0 R	31.0	40.0	32.0	41.0 R	50.0	33.0 R
0.2		0.7836	0.8184	0.9085	0.9832	1.0266	1.1024	1.1359
0.3		1.1091	1.1439	1.2341	1.3087	1.3522	1.4279	1.4613
0.4		1.3243	1.3591	1.4492	1.5246	1.5673	1.6430	1.6765
0.5		1.4771	1.5119	1.6021	1.6767	1.7202	1.7959	1.8293
0.6	1.9542	1.5902	1.6249	1.7151	1.7897	1.8332	1.9089	1.9423
0.8	1.9542	1.7423	1.7771	1.8673	1.9419			
1.0	1.9542	1.8361	1.8709					
1.5	1.9542	1.9542						
2.0	1.9542							
2.5	1.9542							
3.0	1.9542							

c/a	42.0	51.0	60.0 R	43.0	52.0	61.0
0.2	1.1516	1.1958	1.2607	1.2726	1.2955	1.3379
0.3	1.4771	1.5213	1.5863	1.5982	1.6210	1.6634
0.4	1.6923	1.7364	1.8014	1.8133	1.8361	
0.5	1.8451	1.8893	1.9542			

c/a	22.1	31.1 R(13.1)	40.1 R	32.1 R	41.1	50.1 R(05.1)	33.1
0.2	1.1923	1.2062	1.2454	1.2813	1.3037	1.3454	1.3648
0.3	1.3382	1.3590	1.4162	1.4666	1.4973	1.5528	1.5782
0.4	1.4675	1.4927	1.5608	1.6196	1.6548	1.7176	1.7460
0.5	1.5740	1.6021	1.6767	1.7404	1.7782	1.8451	1.8751
0.6	1.6597	1.6895	1.7682	1.8349	1.8743	1.9437	
0.8	1.7828	1.8146	1.8980				
1.0	1.8625	1.8953					

c/a	42.1 R(24.1)	51.1 R	22.2	31.2 R	40.2	32.2 R(23.2)	41.2
0.2	1.3743	1.4012					
0.3	1.5902	1.6247	1.6864				
0.4	1.7595	1.7976	1.7329	1.7468	1.7860	1.8220	1.8444
0.5	1.8893	1.9294	1.7782	1.7959	1.8451	1.8893	1.9165
0.6			1.8192	1.8400	1.8972	1.9476	
0.8			1.8855	1.9108			
1.0			1.9331				

4.7. Precision Measurement of Lattice Parameters of Polycrystalline Specimens

By W. PARRISH and A. J. C. WILSON

4.7.1. Introduction

The precision measurement of lattice parameters by photographic methods has been extensively described by Straumanis and Ieviņš [73], Azároff and Buerger [1], Klug and Alexander [11] (Chapter 8), and Edmunds, Lipson and Steeple [51]. These books should be read for many of the details and additional literature references which cannot be given here. This review deals with the methods used for powder and other polycrystalline specimens and hence is useful mainly for substances of higher symmetry. The application to single crystals is practically identical except that single-crystal goniometers are used, and has the advantage of extending the method to orthorhombic, monoclinic and triclinic substances (see Buerger [3], Farquhar and Lipson [53], and Weisz, Cochran and Cole [80]).

The film methods have been so extensively studied and the techniques are now so well known that lattice parameters can be measured with moderate precision (0.02–0.1%) in routine fashion. The highest credible accuracies reported are usually of the order of 1 part in 50,000 (0.002%), although occasionally there are reports of even higher precision (e.g. Straumanis [74], Weyerer [81]). In principle, the newly developed counter diffractometer should give precision greater than the film methods, but further experience is required to estimate the ultimate accuracy.

There are many factors which contribute to the precision of lattice-parameter measurements, and the methods chosen will depend on the accuracy required for any given problem. There is much discussion in the literature regarding the relative merits of using the most careful experimental techniques (Straumanis [74]) or making mathematical corrections of the experimental data (Cohen [49]). Clearly both approaches must be combined for measurements of the highest accuracy; even in problems requiring only moderate accuracy, reasonably good equipment and careful experimental methods are required in order to apply the mathematical corrections with confidence in the final result.

The general strategy in precision measurements may be outlined as follows: (1) choose the most convenient equipment which is known to give measurements of the accuracy required for the problem; (2) use the most careful experimental technique for instrument alignment, specimen preparation, temperature control, etc., consistent with the time available and the requirements of the problem; (3) wherever possible, use the lines occurring at the higher reflection angles, give them the greatest weight, and select the X-ray wavelengths so that at least one line occurs at $2\theta > 150^\circ$; (4) apply a graphical or mathematical procedure for

dealing with the systematic errors. It would be desirable, of course, first to make some measurements on a few substances whose lattice parameters are known to a high degree of accuracy, in order to check the reliability of the chosen procedure.

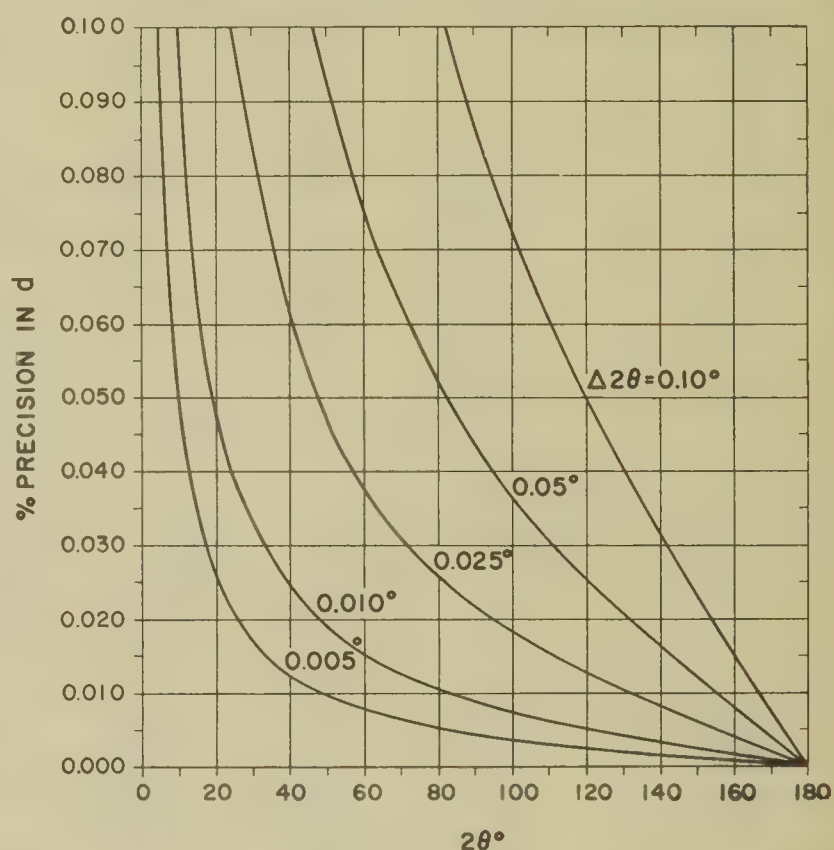


Fig. 4.7.1. Percentage precision of d (spacing measurement) as a function of reflection angles for various errors $\Delta 2\theta$. ($|\Delta d|/d = \cot \theta |\Delta \theta|$.)

In all methods the highest accuracy is normally obtained from lines with the largest reflection angles. The reason for this can be seen by differentiating the Bragg equation, which gives the well-known relation

$$|\Delta d|/d = \cot \theta |\Delta \theta| \quad \dots (1)$$

Fig. 4.7.1 shows the percentage error of the d -spacing measurement as a function of reflection angle for various values of $\Delta \theta$. This is the *minimum* error caused by the limited accuracy with which the reflection angle can be measured. In practice there are usually several sources of systematic errors inherent in the method and equipment which further decrease the accuracy.

4.7.2. Photographic Methods

The three commonest methods for the photographic determination of lattice parameters are based on the use of the cylindrical Debye-Scherrer camera, the symmetrical back-reflection focusing camera, and the back-reflection flat-plate camera. The principal systematic errors inherent in each procedure are described later.

4.7.2.1. DEBYE-SCHERRER METHOD

This method may be further subdivided by reference to the way of mounting the film in the camera according to the method of van Arkel (ends of film in the front-reflection region), Bradley-Jay (ends of film in back-reflection region), or Straumanis (ends of film around $90^\circ 2\theta$). For cameras of the same diameter the three mountings lead to approximately equal accuracy of lattice-parameter determination.

In all film methods the film shrinkage due to processing and ageing is so large that corrections must be made for this factor, and it is usually handled by one of the following procedures, which assume the shrinkage to be uniform along the entire film.

- (a) The Straumanis film mounting has the great advantage of permitting direct measurement of each film in order to obtain the corrections for film shrinkage and effective camera diameter. If there are no lines in the back-reflection region, the Wilson [84] modification of the Straumanis film mounting may be used. For large cameras (diameter $\lesssim 12$ cm.) the Straumanis film mounting requires inconveniently long strips of film.
- (b) The van Arkel and Bradley-Jay film mountings require that the distance between the reference knife-edges be accurately known by a previous independent mechanical or optical measurement.
- (c) Hägg [54] has proposed that a complete scale be printed on the film prior to development.
- (d) Use of a standard substance mixed with the specimen (see Bacon [47] and Andrews [46]). Data for the calculation of reflection angles of standard specimens, such as Al and Si, for several commonly used radiations will be listed in Vol. III of the International Tables.

Absorption in the specimen modifies the line profile and shifts the lines towards higher 2θ . This error decreases with increasing 2θ , and there is a nearly linear relation between line displacement and $\frac{1}{2}\pi - \theta$ for the larger reflection angles. It is one of the commonest sources of systematic error and may be reduced by using a smaller-diameter specimen and/or diluting the specimen with a weakly absorbing non-crystalline substance.

If the specimen rotation axis is not exactly coincident with the film axis and is displaced parallel to the primary beam, the lines will be shifted from their correct position toward higher or lower angles, depending on the direction of this displacement. The error decreases with increasing 2θ . If the displacement is perpendicular to the primary beam it may lead to an incorrect determination of the effective camera diameter in the Straumanis method. Displacement in intermediate directions leads to errors combining these two effects. The camera may be tested for the displacement error (except parallel to the primary beam)

by use of a carefully centred, highly absorbing cylindrical specimen of diameter approximately the same as that of the primary X-ray beam emitted in this direction at the centre of the camera. If the line profiles of the same powder ring on both sides of the direct beam are not identical, the specimen and film axes are not coincident. The error should be minimized by accurate camera construction and careful centring of the specimen.

Divergence of the primary beam in the plane perpendicular to the specimen axis shifts the lines toward higher angles. The error decreases with increasing 2θ . It can be minimized by reducing the angular aperture of the primary beam, or the specimen diameter if the latter is the factor determining the divergence. Divergence of the beam in the plane parallel to the specimen axis (axial or "vertical" divergence†) shifts the back-reflection lines to higher angles and front-reflection lines to lower angles (Lipson and Wilson [58], Easta-brook [50]). Unlike most of the other errors, this error is not eliminated by extrapolation. Fortunately the error is normally very small and may be minimized by decreasing the aperture of the primary beam in the plane of the specimen axis.

Although by using careful experimental technique the width of the reflection can be kept small, there is an unavoidable broadening of the lines in the back-reflection region due to the finite spread of wavelengths in the characteristic radiation. Thus, in measuring the position of a diffraction line, the particular characteristic of the line to be measured must be chosen consistently to minimize subjective errors. It is well known that different observers may choose different points as the position of the line (see for example Ekstein and Siegel [52]), and the same observer may inadvertently use different points on the same film. The differences between the centre of blackening, the centre of intensity (centre of gravity) and the peak intensity are appreciable for precision work. It is difficult to give specific rules for determining the position of a line on a film (see [70]), but this problem is simpler in diffractometer recordings because the entire line profile is available (cf. 4.7.3). For effects of dispersion and of the Lorentz-polarization factor see [70].

The systematic errors of greatest practical importance are listed in Table 4.7.2.1. It will be noticed that to a first approximation all these errors (except knife-edge calibration and axial divergence) vary as $[\frac{1}{2}\pi - \theta]^2$. By plotting the apparent value of the lattice parameter against the function appropriate for the experimental

† Some cameras and diffractometer goniometers are arranged for horizontal operation and others for vertical operation. Thus the term "vertical" divergence is confusing because it may actually be "horizontal," depending on the arrangement of the instrument. The term "axial" divergence is used instead to refer to the divergence parallel to the axis of specimen rotation regardless of whether the camera or goniometer is horizontal or vertical.

TABLE 4.7.2.1
Systematic Errors in the Debye-Scherrer Method

Source of error	Effect on θ^\dagger	Variations of d -error with θ	Remarks
Film shrinkage	+	$(\frac{1}{2}\pi - \theta) \cot \theta$	Affects only van Arkel film mounting without low-angle knife edges.
High-angle knife-edge calibration	+ or -	$\theta \cot \theta$	Affects only Bradley-Jay film mounting. Not eliminated by extrapolation. Requires accurate calibration.
Specimen absorption	+	$\cos \theta \cot \theta$ or $\cos^2 \theta / 2\theta$	Minimized by reducing specimen diameter and/or by dilution.
Specimen displacement			
(a) toward entrance port ..	+	$\cos^2 \theta$	Minimized by accurate camera construction and careful centring of specimen.
(b) toward exit port	-	$\cos^2 \theta$	
(c) sideways	~ 0	~ 0	
Beam divergence			
(a) \perp specimen axis	+	$\cos \theta \cot \theta$ or $\cos^2 \theta / 2\theta$	(a) Decrease collimator aperture or specimen diameter.
(b) \parallel specimen axis	Complex. See equation (11) of Lipson and Wilson [58] and Eastabrook [50].		(b) Decrease length of specimen illuminated. Not eliminated by extrapolation.
Dispersion	See Pike and Wilson [70].		Important at high angles only.

\dagger + = toward higher 2θ , - = toward lower 2θ .

error expected to be largest, the remaining systematic errors will be effectively reduced on linear extrapolation to $\theta = \frac{1}{2}\pi$. The function

$$\frac{1}{2} \left(\frac{\cos^2 \theta}{\sin \theta} + \frac{\cos^2 \theta}{\theta} \right) \quad \dots (2)$$

is found to give good results in practice with linear plots down to small values of θ and has some theoretical justification (Taylor and Sinclair [75]). Values of this function calculated by Nelson and Riley [59] are given in Table 4.7.4A. The function $\cos^2 \theta$ is also useful, and values may be obtained from Table 4.7.4B.

The importance of careful experimental technique has been stressed by Straumanis [73] [74]. Film shrinkage is determined by direct measurement of the film; careful centring and accurate camera construction reduce specimen eccentricity; small-diameter specimens are used to obtain sharp lines; absorption errors are reduced by the small-diameter specimen and dilution when required; accurate temperature control is maintained during the exposure; radiation is chosen to give one or more very-high-angle reflections;

and finally the film is measured with a precision device. Straumanis claims that systematic errors are eliminated by the careful experimental technique and he does not use an extrapolation method. However, even when all these precautions are taken, there are probably some systematic errors remaining. For example, it is not possible to obtain good reflections from highly absorbing materials which have been diluted to the point where the absorption error is negligible. The importance of careful experimental procedures is that the systematic and random errors are reduced and there is greater confidence in the measurements.

4.7.2.2. SYMMETRICAL BACK-REFLECTION FOCUSING METHOD

In this method measurements are more conveniently expressed in terms of the complement of θ :

$$\phi = \frac{1}{2}\pi - \theta \quad \dots (3)$$

The corrections for film shrinkage are usually done by means of previously calibrated knife-edges on the low-angle ends of the film. Some cameras are also equipped with high-angle knife-edges and a number of equally

4.7. PRECISION MEASUREMENT OF LATTICE PARAMETERS OF POLYCRYSTALLINE SPECIMENS

spaced notches on the circumference of the camera to make certain that differential film shrinkage has not taken place. Standard substances mixed with the specimen are sometimes used for calibration. Errors due to penetration of the beam into low-absorbing specimens may be minimized by the use of very thin samples, longer wavelengths, or both. Care must be exercised in specimen preparation to make certain the specimen has the correct curvature and that its front surface lies on the same circle as the front surface of the film. Divergence of the primary beam in the plane normal to the camera diameter (axial divergence) should be kept small, since errors due to shifts of lines from this cause increase with decreasing ϕ . Good camera construction is required to minimize errors due to displacement of the entrance slit from the focusing

circle, to obtain parallelism of the knife-edges, to ensure good contact of the film round the focusing circle and to reduce errors from similar factors. Double-coated film gives images on the two sides which do not coincide. The back image should therefore be stripped or its development prevented, for example by an adhesive strip which is removed prior to fixing [64]. Single-coated film is more convenient but is usually slower and not easy to obtain.

The systematic errors are listed in Table 4.7.2.2. To a first approximation all the errors listed (except axial divergence) vary as ϕ^2 , and $\phi \tan \phi$ appears to be the most acceptable extrapolation function. A linear plot is used for all lines with $\phi \lesssim 30^\circ$. Values of $\phi \tan \phi$ are given in Table 4.7.4C. (See also Saini [72], Jette and Foote [56], and Cohen [49].)

TABLE 4.7.2.2
Systematic Errors in the Symmetrical Back-reflection Focusing Method

Source of error	Effect on ϕ^\dagger	Variations of d -error with ϕ
Film shrinkage	—	$\phi \tan \phi$
Low-angle knife-edge calibration	+ or —	$\phi \tan \phi$
Specimen transparency	+	$\tan^2 \phi$
Specimen displacement		$\tan 2\phi \tan \phi$
(a) Outside true circumference	+	
(b) Inside true circumference	—	
Beam divergence in plane \perp to camera diameter ..	+	$\tan 2\phi \tan \phi$

\dagger + = toward larger ϕ , — = toward smaller ϕ . ($\phi = \frac{1}{2}\pi - \theta$.)

TABLE 4.7.2.3
Corrections to Measurements with Flat-plate Back-reflection Camera †

Source of error	Correction
Film shrinkage	Use low-angle knife-edges or other fiducial marks.
Specimen-to-film distance	Use accurate mechanical gauge or calibrating substance.
Specimen transparency	Decrease D by $2 \tan 2\phi / \mu(1 + \sec 2\phi)$, or use thin specimen or longer wavelength.
Inclination of incident beam to specimen normal	Construct camera so that inclination of central ray is less than 0.1° .
Beam divergence	Limit to small values or reduce D by $\frac{3}{8} D \tan^2 \alpha$.

\dagger D = measured ring diameter, $\phi = \frac{1}{2}\pi - \theta$, μ = linear absorption coefficient, α = semi-angle of divergence.

4.7.2.3. FLAT-PLATE BACK-REFLECTION METHOD

The small number of lines recorded by a flat-plate camera ordinarily makes extrapolation techniques impractical. If accurate lattice parameters are required by this method, accurate instrument construction and careful calibration are required. The principal corrections are listed in Table 4.7.2.3. The corrections can be minimized by coating the surface of the specimen with a thin film (~ 0.002 cm thick) of a calibrating substance such as aluminium or silver and measuring one ring from the standard and one from the substance under investigation. The angle ϕ is then found from the relation

$$\tan 2\phi = (D/D_c) \tan 2\phi_c \quad \dots (4)$$

where D_c and ϕ_c refer to the calibrating substance. For best results the standard should be chosen so that D_c is nearly equal to but slightly greater than D . In calculating ϕ_c allowance must be made for the variation of d_c with temperature. The double coating of the film again leads to displaced images, and this error should be eliminated, as mentioned in the previous section. Great care must be taken to prevent buckling of the film. (See also Thomas [77] and Edmunds, Lipson and Steeple [51].)

4.7.3. Counter-diffractometer Method

The following description of this relatively new method applies to focusing instruments employing counter-tube detectors, such as Geiger, proportional or scintillation counters (Parrish and Hamacher [60]). At the time of writing very little has been published on the application of the method to precision lattice-parameter measurements, and it is likely that this survey will require some modifications during the next decade. The possible major sources of errors are reviewed below and listed in Table 4.7.3. These generally have their origin in the geometrical aberrations caused by limitations of the practical X-ray optical system, improper specimen preparation, imperfections in the goniometer, its alignment and calibration, and limited accuracy of the intensity measurements.

The precise alignment of the counter diffractometer can be made with simple mechanical devices (Parrish and Lowitzsch [63]). This is important not only to obtain the highest intensity and best resolution but also to minimize errors due to geometrical aberrations caused by several possible small misalignments, such as inequality of source-specimen and specimen-receiving-slit distances, small errors in the counter tube (2θ) : specimen (θ) setting, commonly called the 2 : 1 setting; and so on.

These aberrations are further minimized by setting the centre of gravity of the primary beam (rather than the geometrical middle of the irradiated specimen length) on the goniometer axis of rotation. This reduces residual misalignment errors and profile distortions due to non-uniform intensity of the primary beam and variations in the length of specimen irradiated at

different Bragg angles. The zero-angle calibration is done with a knife-edge (Tournarie [78]) or pinhole (Parrish and Lowitzsch [63]) placed in the specimen holder and scanning the direct beam, preferably at small angular steps. The accuracy may be as great as $\pm 0.001^\circ 2\theta$. The techniques of using Geiger, proportional and scintillation counters have been reviewed recently, with emphasis on linearity, efficiency, pulse-amplitude discrimination, counting statistics and related topics [65, 66].

The best focusing is obtained when the specimen surface is curved in the form of a section of a cylindrical surface to fit the focusing circle. The radius of the focusing circle r decreases with increasing Bragg angle θ according to the relation

$$r = R/2 \sin \theta \quad \dots (5)$$

where R is the radius of the goniometer. Hence the specimen would have to be prepared in a flexible mount whose curvature could be accurately and continually varied in synchronism with the movement of the receiving slit. This is difficult to do in practice, and flat specimens are normally employed.

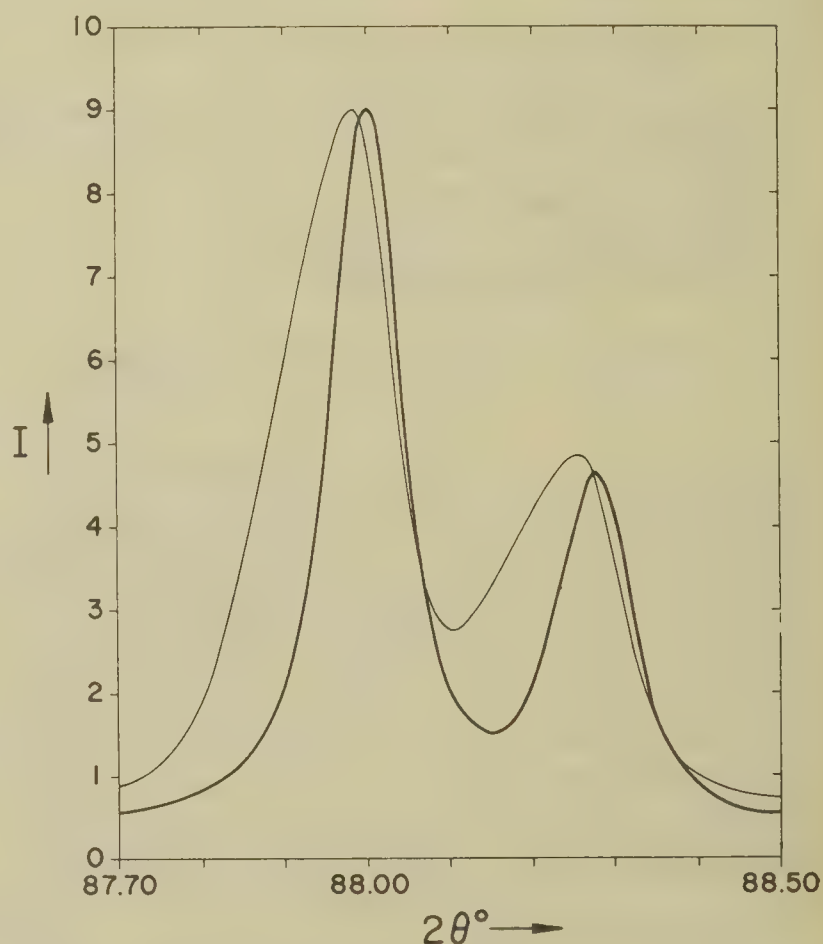


Fig. 4.7.3(1). Flat specimen aberration shown by change of intensity (I) distribution. Profiles replotted from step-scan recording at $0.01^\circ 2\theta$ steps, probable error 0.8% (6400 counts), angular aperture $2\alpha = 1^\circ$ (darker line), $2\alpha = 4^\circ$ (lighter line) and normalized for equal peak intensity of $K\alpha_1$. Silicon powder specimen (422), $\text{CuK}\alpha$, two sets of parallel slits each with angular aperture $4^\circ 35'$, receiving slit $0.05^\circ 2\theta$, $R = 17$ cm.

TABLE 4.7.3
Sources of Major Errors in Counter Diffractometry

Source of error	Maximum effect on reflection angle at	Direction of shift (2θ) [†]		Variation with θ of		Remarks
		0–90°	90–180°	2θ	d	
Instrument misalignment ..						Minimize by careful alignment and centre c.g. of primary beam on axis of rotation.
2:1 mis-setting ..					~0	Causes asymmetric broadening, little effect on c.g., small shift of peak to higher 2θ. Eliminated by careful alignment.
Zero-angle calibration ..		+ or –	+ or –	Constant	cot θ	Requires accurate mechanical calibration with pinhole or knife-edge. d error not linear.
Flat specimen ..	Small 2θ (α constant) 90° 2θ (L constant)	–	–	cot θ	cot ² θ	Causes asymmetrical broadening toward small 2θ. Extrapolates to zero.
Transparency ..	90° 2θ	–	–	sin 2θ	cos ² θ	Same as for flat specimen. Reduce by use of thin specimens of materials with small absorption.
Axial divergence ..	Small and large 2θ	Complex: – at small angles, + at large angles				Extrapolates to a constant. Minimize by use of small 2δ. [‡] See p. 223 and [67].
Specimen displacement ..	Small 2θ	+ or –	+ or –	cos θ	cos θ cot θ	Usually source of largest error but extrapolates to zero. Minimize by careful specimen preparation.
Rate-meter recording ..		+ or –	+ or –	Constant	cot θ	Time constant and scan speed cause asymmetric broadening and shift of c.g. and peak towards scanning direction. Eliminated by fixed-count intensity measurements and reduced by use of small time constant and scan speed.
Dispersion and Lorentz factor	Large 2θ	Negligible	+	tan ³ θ	tan ² θ	Largest error in c.g. at very high 2θ. Does not extrapolate to zero. Little effect on peak.

[†] + = toward higher 2θ; – = toward lower 2θ.[‡] δ = tan s/l, where s = spacing, l = length of Soller slits.

The use of a flat specimen gives rise to small geometrical aberrations which broaden the line profile asymmetrically and shift the position of the reflection to smaller angles, as shown in Fig. 4.7.3(1). In addition, penetration of the primary beam into specimens of low absorption and reflections from below the surface (transparency error) produce similar aberrations. Wilson [85] has developed the following expression for the shift of the centre of gravity (c.g.)† of the diffraction maximum to smaller angles (expressed in 2θ radians) due to these two aberrations:

$$\Delta 2\theta_{\text{(c.g., rad.)}} = -\frac{L^2 \sin 2\theta}{12R^2} + \frac{\sin 2\theta}{2\mu R} - \frac{2t \cos \theta}{R[\exp(2\mu t \csc \theta) - 1]} \quad \dots (6)$$

where L is the length of specimen illuminated ($L = 2\alpha R / \sin \theta$, 2α is the full angular aperture of the primary beam in the plane of Bragg focusing), μ the linear absorption coefficient and t the specimen thickness. The first term, due to the flat specimen, is plotted in Fig. 4.7.3(2) for various values of 2α , $R = 17$ cm, with $\Delta 2\theta$ expressed in degrees. The shift increases with 2α and falls to zero at $180^\circ 2\theta$, giving rise to a systematic error. The parabola is for the case $L = 2$ cm for all θ 's (2α increasing with θ).

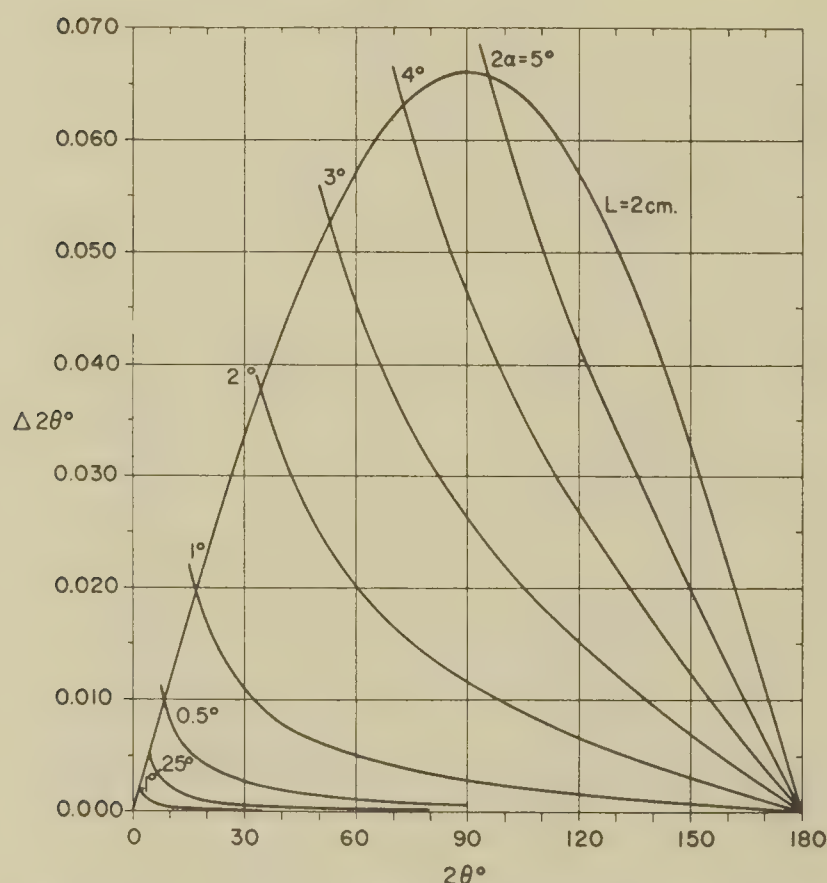


Fig. 4.7.3(2). Shift of centre of gravity due to flat-specimen aberration ($L^2 \sin 2\theta / 12R^2$; $R = 17$ cm) for various values of 2α .

The second and third terms of equation (6) give the shift due to specimen transparency. In most practical cases $\mu t \csc \theta$ is large, so that the third term drops out. Fig. 4.7.3(3) shows a plot of the second term for various values of μ . The shift is greatest at $90^\circ 2\theta$,

falling to zero at 0° and $180^\circ 2\theta$, and is another source of systematic error. It should be noted that high specimen absorption is usually the source of largest error in the Debye-Scherrer method, whereas low specimen absorption may cause major aberrations in the focusing methods.

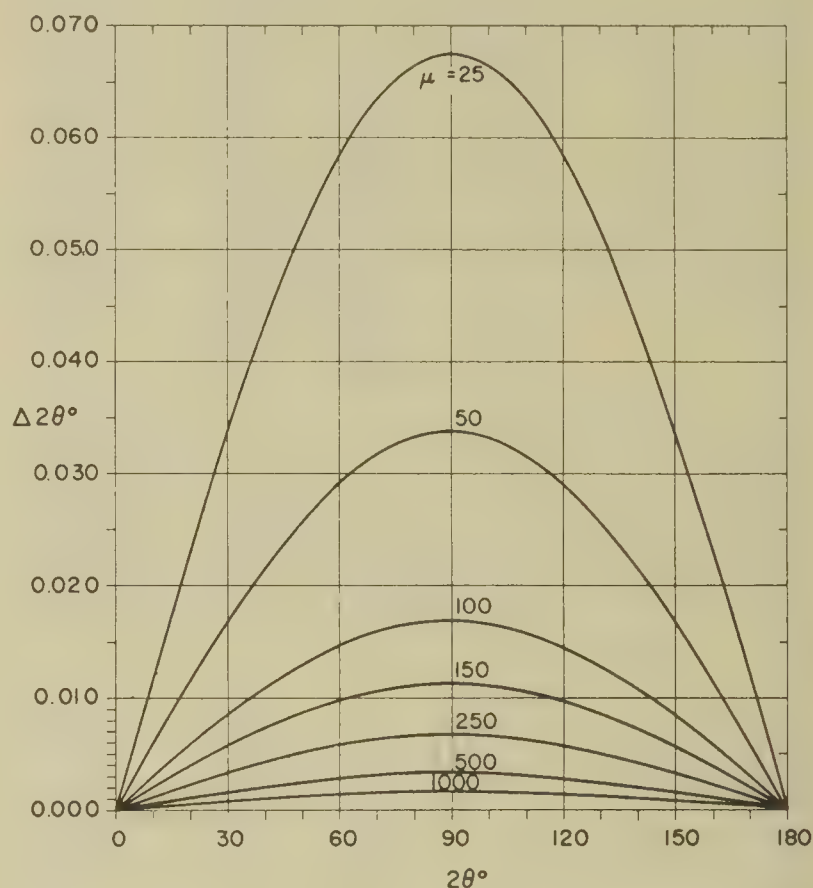


Fig. 4.7.3(3). Shift of centre of gravity due to specimen-transparency aberration ($\sin 2\theta / 2\mu R$; $R = 17$ cm) for various values of μ .

The effects of these aberrations on the peak position are more difficult to derive, and Wilson [85] gives a solution which is probably satisfactory for the smaller angles $0^\circ < 2\theta < 40^\circ$. The shift of the peak to smaller 2θ expressed in radians is given by the *smallest* value of the three expressions

$$\Delta 2\theta_{\text{(Peak, rad.)}} = \left. \begin{aligned} &= L^2 \sin 2\theta / 4R^2 & (a) \\ &= 0.428 \sin 2\theta / \mu R & (b) \\ &= 2t \cos \theta / R & (c) \end{aligned} \right\} \quad \dots (7)$$

where the symbols have the same meaning as above. In most practical cases expression (7b) is dominant. For example, at $2\theta = 20^\circ$, $L = 2$ cm, $\mu = 100$, $t = 0.1$ cm, the shifts in degrees 2θ are 0.068° , 0.005° and 0.664° for equations (7a), (b), (c) respectively.

† There is some difference of opinion as to whether it is possible to define the position of the *centre of gravity* of a diffraction maximum (especially if it has long "tails") with sufficient exactness to warrant the use of this position as representing the true or, at least, a reproducible location of the diffraction maximum. The authors claim that the "tails" do fall off rapidly enough for the centre-of-gravity position to be used, at least in the case of well-crystallized polycrystalline specimens and a diffractometer of good resolution, and that no other measure is at present suitable for accurate work.—GENERAL EDITOR.

The divergence of the primary beam perpendicular to the plane of Bragg focusing, sometimes called the axial divergence, is limited in the newer diffractometers by thin parallel slits (Soller slits). Usually one set is placed between the source and specimen and another set between the specimen and counter detector. These slits are required to obtain good line shape at small and large diffraction angles with an extended line source of X-rays. Increasing the axial divergence broadens the line asymmetrically as shown in Fig. 4.7.3(4), and shifts the peak and c.g. of the reflection in a complex manner. The peak shift is usually less than that of the c.g.

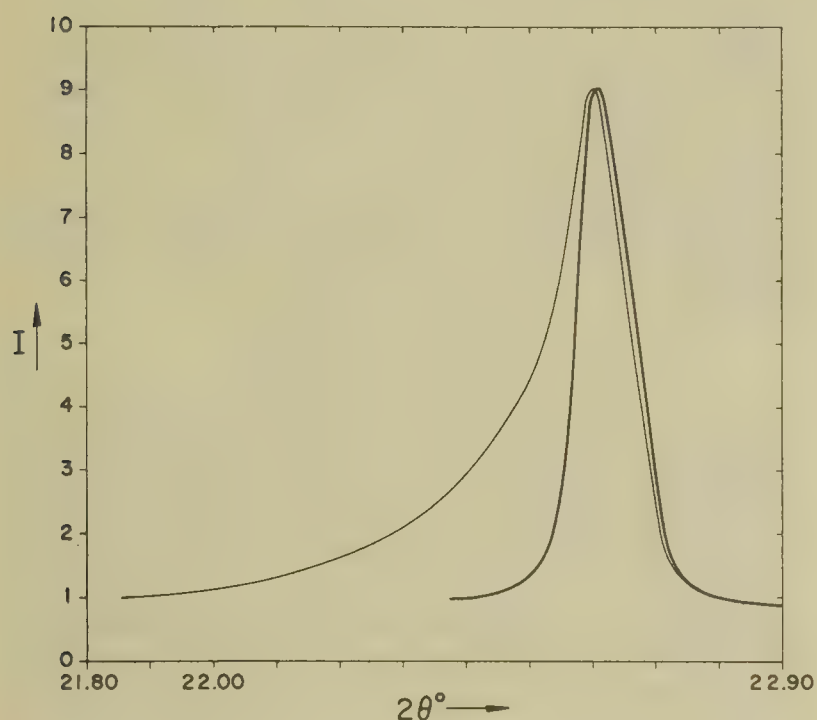


Fig. 4.7.3(4). Change in line profile caused by increasing divergence of beam in plane of parallel slits. Curves normalized for equal peak intensity. Heavy line profile obtained with one set of parallel slits between source and specimen, one set between specimen and detector, each having angular aperture $2^\circ 18'$. Light line obtained with slits removed and angular aperture limited by specimen width to approximately 6.5° . Lead nitrate curved powder specimen, $\text{CuK}\alpha$ (200), $r=43.3$ cm, $2\alpha=1^\circ$, receiving slit $0.05^\circ 2\theta$, $R=17$ cm.

The shift is toward smaller angles in the front-reflection region, but changes sign in the region 90° to $120^\circ 2\theta$, above which the shift is toward larger angles. The magnitude of the shift and the angle at which the shift changes sign have no simple expression but depend in a complicated way on the axial lengths of source, specimen and receiving slit, and whether one or two (or no) sets of parallel slits are employed. Eastabrook [50] has considered the limiting case when the spacing of the parallel slits is small. Pike [67] has given a fuller theoretical treatment and presents data for shifts that occur under various experimental conditions.

If the surface of the specimen is displaced a distance S from the goniometer axis of rotation, the peak and c.g. of the reflection are both shifted by

$$\Delta 2\theta = 2S \cos \theta / R \quad \dots (8)$$

(Peak, c.g., rad.)

to higher angles if the specimen is inside the focusing circle, and to lower angles if outside (Wilson [85]). The shift decreases with increasing reflection angle, becoming zero at $2\theta=180^\circ$, and thus can be eliminated by extrapolation. The displacement may be caused by inaccurate machining of the banking surface of the specimen holder of the goniometer, and hence is a constant of the instrument and/or the specimen preparation; in the latter case it varies from one specimen to another. A shift may also occur if the surface of the specimen is not planar or if the specimen surface is not parallel to the goniometer axis.

The finite width of the source and receiving slit have no effect on the c.g. of the reflection and only broaden the line. Where the maxima are unsymmetrical, as in the case of $\text{K}\alpha_1-\alpha_2$ doublets, a narrow receiving slit will give the "true" peak position but a wide slit may cause the peak to shift toward the centre of gravity of the two lines. If receiving slits with different widths are used, the zero-angle calibration must be made with the slit actually in use. Ordinarily different slits will give somewhat different angles, because of the difficulty of making the distance between the centre of the slit opening and the reference surface exactly the same from one slit to another.

From this summary it appears that for most of the errors in counter diffractometry, except axial divergence, the extrapolation function is either $\cot \theta \cos \theta$ or $\cos^2 \theta$, depending on whether the specimen surface displacement or flat specimen and transparency error is larger. Extrapolation may be avoided by the procedure described below, but the difficulty of measuring the surface displacement S makes extrapolation desirable for many specimens.

In counter diffractometry the accuracy of the angular measurements is dependent on the accuracy of the intensity measurements. In routine analysis with a rate-meter and strip-chart recorder, the peak and c.g. of the lines are shifted toward the scanning direction by an amount dependent on the product of the scanning speed of the goniometer and time constant of the circuits (Parrish [62]; Tournarie [79]; Parrish and Hamacher [60]). For example, if this product is increased from 1 to 32 the shift increases nearly linearly from 0.01° to $0.10^\circ 2\theta$ in a typical practical case. The amount of shift is also dependent on the line shape and width of the receiving slit. This electronic aberration can be the source of a large error, and in work of higher precision it is desirable to eliminate this error by the use of a step-scanning method. The steps should be small compared to the line breadth, and normally steps of 0.01° to $0.05^\circ 2\theta$ are used. A fixed-time or fixed-count (preselected

probable error) intensity measurement can be used. The former has the advantage of requiring much less time and gives sufficient precision if a reasonable number of counts is obtained at each step. The time required to record the entire profile may be greatly reduced by using larger steps (and/or reducing the fixed count) in the tails. If the detector is non-linear, the intensities must be corrected. It is often easier to determine the approximate integration limits from a preliminary rapid rate-meter recording.

It has been shown above that the geometrical aberrations have been worked out only for the c.g. (centroid or first moment) of the line profile. The observed distribution is a convolution of the spectral distribution and the aberrational distributions. Since the c.g.'s of the individual aberrations are additive, it is easy to subtract the effect of their displacements of the line profile and thus obtain the c.g. of the angular representation of the spectral distribution $h(\theta)$. In cases where the dispersion is not too great, the c.g. of the spectral distribution on an angle scale then corresponds to the c.g. on a wavelength scale $h(\lambda)$, and the Bragg equation

$$d = n\tilde{\lambda} / \sin \tilde{\theta} \quad \dots (9)$$

yields the interplanar spacing where $\tilde{\lambda}$ and $\tilde{\theta}$ refer to the c.g.'s of the spectral distribution. $\tilde{\lambda}$ is defined as

$$\tilde{\lambda} = \frac{\int \lambda h(\lambda) d\lambda}{\int h(\lambda) d\lambda} \quad \dots (10)$$

The range of the integrals in equation (10) should be over the whole recorded spectrum. It is impractical to work with such limits because the tails of spectral lines decay too slowly and for other obvious reasons. This difficulty is overcome by truncating the distribution in a manner that preserves its basic features. To maintain the correspondence of the spectral and observed distributions, the latter is truncated in the same manner. The c.g. of the observed distribution, assuming negligible dispersion, is

$$\tilde{\theta} = \frac{\int \theta h(\theta) d\theta}{\int h(\theta) d\theta} \quad \dots (11)$$

Two truncation methods have been proposed and tested in a limited manner:

(i) Pike and Wilson [69] define arbitrary limits in the tails of the spectral profile, make a "horizontal" truncation between them and use the c.g. of the truncated "line" as $\tilde{\lambda}$ in the Bragg equation. The correspondence of the spectral and observed distributions is ensured by finding the value of d which transforms the limits and the c.g. of this "line" to points on the observed distribution which have the same property, i.e. the observed c.g. is that of the truncated distribution between the observed limits. Such a value of d is found by successive approximations. The effects of geometrical aberrations, dispersion, and the Lorentz-polarization factor are allowed for in the comparison.

A simplified procedure is described which is valid for angles which are not too high ($>140^\circ 2\theta$), or too low ($<60^\circ 2\theta$). For this procedure the limits are chosen symmetrically about the c.g. by successive approximations on both λ and θ scales, and the exact range used is not critical, provided it is sufficiently large.

(ii) Ladell, Parrish and Taylor [57] preserve the basic features of the distribution by neglecting part of the tails. The integrated intensity is measured and a line is drawn parallel to the background line so that the area between the lines is about 10% of the total integrated intensity. The limits are taken as the abscissae where the upper line intersects the profile and the c.g. is calculated between these limits. Thus only 2–3% of the entire distribution is neglected.

The error of approximation in both procedures is small compared with the measurable diffractometer error ($<0.001^\circ 2\theta$) at angles important for lattice-parameter determination.

Where dispersion $d\theta/d\lambda$ is significant (say $>125^\circ 2\theta$), and other aberrations are small, the angle which is equivalent to $\tilde{\lambda}$ is given by θ_B where

$$\theta_B = \sin^{-1} \left\{ \frac{\int (\sin \theta) h(\theta) d\theta}{\int h(\theta) d\theta} \right\} \quad \dots (12)$$

In practice the c.g. of the observed distribution $I(\theta)$ is reduced to $\tilde{\theta}$, the c.g. of the spectral distribution, by subtracting the known displacements due to the aberrations. θ_B is then determined by adding the displacement due to dispersion, $\theta_B - \tilde{\theta}$, which has been calculated for several known spectral distributions [57] and from approximate models of spectral distributions [68]. The interplanar spacing is then determined by

$$d = n\tilde{\lambda} / 2 \sin \theta_B \quad \dots (13)$$

The important part of the Lorentz factor, $1/\cos \theta$, also changes rapidly in this region and its effect must be subtracted in high-precision work. The combination of dispersion and Lorentz factors distorts the profile and shifts the c.g., but the peak position is very much less affected. Pike [68] gives for the combined effect of dispersion and the Lorentz factor the general expression

$$\Delta 2\theta = \frac{3V}{\tilde{\lambda}^2} \tan^3 \tilde{\theta} \quad \dots (14)$$

(c.g., rad.)

where V is the variance (mean-square breadth) of the spectral profile over the range actually used in the centre-of-gravity determination. Neither the dispersion nor the Lorentz corrections extrapolate to zero, and, in fact, they become the largest source of error at very high 2θ . Other trigonometrical factors produce a very small shift of the c.g. at very high angles.

A procedure which eliminates extrapolations and is based on the principles described above has been used successfully [57]. All the individual aberrations for the particular experimental conditions are added and a plot is made of the shift of c.g. against 2θ . The

observed c.g.'s of the lines in the back-reflection region are then corrected from the plotted aberrational data yielding d values free of systematic errors. The numerical average (without weighting) of these d 's is calculated to reduce the effects of random errors. This average d is then corrected for the usual factors such as temperature and refraction to obtain the final d . This procedure works only when all the significant aberrations are known, and hence is applicable at present only to c.g. measurements of the lines. In the case of $\text{CuK}\alpha$ radiation, silicon powder, $2\alpha=4^\circ$, two sets of parallel slits each with 4.5° aperture, the geometrical aberration correction is -0.045° at $105^\circ 2\theta$ and -0.001° at $160^\circ 2\theta$.

There are several advantages (a) and disadvantages (b) in using the c.g. rather than the peak position.

(a) The c.g. is a more accurate determination of the reflection maximum, since it is based on many points across the entire line profile rather than the few points around the peak. It gives an accurate measurement regardless of the $\text{K}\alpha$ doublet separation, line asymmetry or breadth, whereas there is always some doubt in the choice of the peak position in these cases. The corrections required for certain geometrical aberrations can be most easily expressed in terms of the c.g., but the expressions for the shift of peak position are known accurately for only a few limited conditions. It is preferable to work with a displacement of the c.g. whose angular variation is known, rather than the displacement of the peak whose angular variation is unknown, even if the latter is somewhat smaller. The unfolding operation to eliminate errors is reduced to a simple subtraction.

(b) The measurement of the c.g. takes a great deal more time than the peak and is desirable only in cases where high accuracy is required. Since the broadening of the lines due to the aberrations mentioned earlier is usually asymmetric, the c.g. is usually more sensitive than the peak and hence has a larger systematic error. In the lower-symmetry substances overlapping of lines may make it impossible to measure the c.g. It is also likely that when the diffractometer is better understood through studies of the c.g. method, some empirical methods of using peaks with high precision may be discovered.

4.7.4. General Problems

(a) *Extrapolation.* Many of the errors vary in a systematic fashion, decreasing with increasing reflection angle, and hence some form of extrapolation is often desirable. Since not all the errors conform to any one function, the choice of the function depends on a knowledge of the relative importance of each source of error for any given method. The most likely functions for each method have been described above, but these may require modification, depending on the special characteristics of the experimental conditions.

The accuracy of the extrapolation depends on the presence of several well-spaced good lines in the back-reflection region with one or more above $160^\circ 2\theta$, and the magnitude of the random as well as the systematic errors. There are two general approaches to extrapolation: graphical (Bradley and Jay [48]) and analytical—based on the least-squares method (Cohen [49]; Hess [55]). The advantage of the graphical method is its simplicity and the ease with which the highest-angle determinations or those with the most favourable indices (see below) may be weighted.

For cubic crystals the simplest and probably best method of extrapolation is to plot the apparent value of the lattice parameter a against the chosen extrapolation function and draw the best extrapolation line through the points to $180^\circ 2\theta$ with the aid of a transparent straight-edge. Tables of $\frac{1}{2}(h^2+k^2+l^2)^{\frac{1}{2}}\lambda$ are available to facilitate the calculation of the provisional a for each reflection (Parrish, Ekstein and Irwin [61]). For tetragonal and hexagonal crystals the same method may be used with the following modification. An approximate value for the axial ratio is chosen, the values of a are calculated from lines with low l index and c from lines with low h and k indices (Wilson and Lipson [83]). If the axial ratio of the extrapolated values differs significantly from that chosen the process is repeated, and the final axial lengths are thus found by one or more steps of successive approximation. If only one (001) reflection is present, the method of Taylor and Floyd [76] may be useful.

The selection of a fairly good value of the axial ratio may be facilitated by measuring a pair of lines at moderately high 2θ angles with good experimental technique (Straumanis [74]; Klug and Alexander [11]). If h_1, k_1, l_1, θ_1 refer to one reflection and h_2, k_2, l_2, θ_2 to the other, we may combine the quadratic forms of the Bragg equations for each reflection and obtain for tetragonal crystals

$$a = \frac{\lambda}{2} \left[\frac{l_1^2(h_2^2 + k_2^2) - l_2^2(h_1^2 + k_1^2)}{l_1^2 \sin^2 \theta_2 - l_2^2 \sin^2 \theta_1} \right]^{\frac{1}{2}} \dots (15)$$

from which c may be calculated from any reflection

$$c = \lambda a l [4a^2 \sin^2 \theta - \lambda^2(h^2 + k^2)]^{\frac{1}{2}} \dots (16)$$

For hexagonal crystals the corresponding expressions are

$$a = \lambda \left[\frac{l_1^2(h_2^2 + h_2k_2 + k_2^2) - l_2^2(h_1^2 + h_1k_1 + k_1^2)}{3(l_1^2 \sin^2 \theta_2 - l_2^2 \sin^2 \theta_1)} \right]^{\frac{1}{2}} \dots (17)$$

$$c = \frac{\lambda a l}{2} \left[\frac{3}{3a^2 \sin^2 \theta - \lambda^2(h^2 + hk + k^2)} \right]^{\frac{1}{2}} \dots (18)$$

If the two reflections were obtained with different wavelengths ($\alpha_2, \alpha_1, \beta$ or another target), equation (15) may be modified to

$$a = \frac{\lambda_1 \lambda_2}{2} \left[\frac{l_1^2(h_2^2 + k_2^2) - l_2^2(h_1^2 + k_1^2)}{\lambda_1^2 l_1^2 \sin^2 \theta_2 - \lambda_2^2 l_2^2 \sin^2 \theta_1} \right]^{\frac{1}{2}} \dots (19)$$

and equation (17) to

$$a = \lambda_1 \lambda_2 \left[\frac{l_1^2(h_2^2 + h_2 k_2 + k_2^2) - l_2^2(h_1^2 + h_1 k_1 + k_1^2)}{3(\lambda_1^2 l_1^2 \sin^2 \theta_2 - \lambda_2^2 l_2^2 \sin^2 \theta_1)} \right]^{\frac{1}{2}} \quad \dots (20)$$

The graphical and analytical methods become more difficult to use as the crystal symmetry decreases, and generally single-crystal methods are easier for orthorhombic and lower-symmetry substances. In orthorhombic crystals

$$\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2} = \frac{1}{d^2} \quad \dots (21)$$

so that if the extrapolation function appropriate to d is $f(\theta)$:

$$\frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{l^2}{c^2} - \frac{4 \sin^2 \theta}{\lambda^2} = K \sin^2 \theta f(\theta) \quad \dots (22)$$

where K is a constant for a particular set of measurements. This equation has four adjustable constants a , b , c , K ; and the best values can be found by the usual least-squares methods. Values of $\sin^2 \theta$ are given in Table 4.7.4B. Five-figure tables of $\sin^2 \theta$ for every hundredth of a degree from 2° to 87° have been prepared by H. Anne Plettinger [71]. Equation (22) can be modified for crystals of higher or lower symmetry.

The analytical method can be extended to cover cases where there are important errors with different dependence on θ . The right-hand side of equation (22) is replaced by

$$\sin^2 \theta [K_1 f_1(\theta) + K_2 f_2(\theta) + K_3 f_3(\theta) + \dots] \quad \dots (23)$$

and K_2 , K_3 are treated as additional adjustable constants in the least-squares solution. Experimental accuracy is rarely sufficiently great to make this worth while, but if there is doubt about the high-angle knife-edge calibration of a Bradley-Jay camera or the zero-angle calibration of a diffractometer, a term with $f_2(\theta) = \theta \cot \theta$ or $\cot \theta$ respectively might be included.

(b) *Thermal Expansion.* The lattice parameter a varies with the coefficient of thermal expansion α and temperature T according to the relation

$$a_{T_2} = a_{T_1} + \alpha a_{T_1} (T_2 - T_1) \quad \dots (24)$$

The values for α may range from a few parts to nearly 100 parts per million per degree C. Some representative approximate values of $10^6 \alpha$ are tungsten 4, sodium chloride 40, thallium chloride 55. It is therefore necessary to control the temperature of the specimen to well within the limits set by the desired precision of the lattice-parameter measurement. Small fluctuations around the desired temperature cause a small symmetrical broadening of the lines on film. A longer-range gradual change in temperature causes unsymmetrical broadening on film and may lead to a systematic error in counter diffractometry.

(c) *Refraction.* The wavelength of X-rays within a crystal (λ') differs slightly from that in air (λ). The observed reflection angle (θ') is different, therefore, from the θ calculated from the Bragg equation, for two reasons: (i) λ' is slightly larger than λ , (ii) the X-rays are changed slightly in direction due to refraction on entering and leaving the crystal. In the case of small, roughly spherical crystals with negligible absorption, the second effect is equally likely to cause an increase or a decrease in reflection angle and hence causes only a slight line broadening. Thin plates or needles require a special correction. Ordinarily in powder work only the first effect has to be considered (Wilson [82]). Either the corrected wavelength $\lambda' = \lambda/N$ (where N is the index of refraction) may be used in calculating d from θ , or, as is the commonest practice, d' calculated with refraction neglected may be increased by

$$(1 - N)d' = 2.70 \times 10^{-6} \lambda^2 \rho d \Sigma Z / \Sigma A \quad \dots (25)$$

which for cubic crystals may be put in the more convenient form

$$(1 - N)a' = 4.48 \times 10^{-6} (\lambda/a)^2 \Sigma Z \quad \dots (26)$$

In these equations λ is in Å and ρ in g/cm³; ΣZ is the sum of the atomic numbers and ΣA the sum of the atomic weights of the atoms in the unit cell. The correction is usually small (a few parts to be added to the lattice parameter in the fifth decimal place). Some typical values of $(1 - N)a' \times 10^6$ are:

	MoK α	CuK α	CrK α
Aluminium ..	7.2	33.7	74.4
Lead nitrate ..	21.1	99.1	219.0
Tungsten ..	33.4	157.0	347.0

(d) *X-ray Wavelengths.* Due to continuing uncertainty concerning the precise *absolute* values of X-ray wavelengths, it is recommended that the values used in precision measurements should be explicitly stated. Confusion arises from three sources: (i) uncertainty in the value of the factor for converting kX to Å units, (ii) limited and variable precision in the original determinations of the wavelengths, and (iii) the asymmetric spectral distribution of the small band of wavelengths comprising the "monochromatic" X-rays, which may cause the peak value to differ from the centre of gravity or any other type of weighted mean.

The existing state of knowledge concerning absolute X-ray wavelengths and the conversion factor will be discussed in Volume III. Meanwhile it may be pointed out that, if spacings of the highest precision are required, peak measurements of *diffraction maxima*

4.7. PRECISION MEASUREMENT OF LATTICE PARAMETERS OF POLYCRYSTALLINE SPECIMENS

should be combined with peak measurements of *wavelength*, or centre-of-gravity measurements with centre-of-gravity measurements, and so on. Whatever method of location of exact intensity maxima is used, it should be the same in each case. This may involve further consideration of the methods that have hitherto

been used to locate wavelength maxima, especially as information concerning the method employed is not always clearly given in the literature; and in the case of $\text{CuK}\alpha$, for example, there is a difference of about 0.0045% between the c.g. of the α_1 and α_2 components and the weighted mean of the peak wavelengths [57].

4.7, PRECISION MEASUREMENT OF LATTICE PARAMETERS OF POLYCRYSTALLINE SPECIMENS

TABLE 4.7.4A

$$\frac{1}{2} \left(\frac{\cos^2 \theta}{\sin \theta} + \frac{\cos^2 \theta}{\theta} \right)$$

θ°	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
10	5.571	5.513	5.456	5.399	5.344	5.290	5.237	5.185	5.134	5.084
11	5.035	4.986	4.938	4.892	4.846	4.800	4.756	4.712	4.669	4.627
12	4.585	4.544	4.504	4.464	4.425	4.386	4.348	4.311	4.274	4.238
13	4.202	4.167	4.133	4.098	4.065	4.032	3.999	3.967	3.935	3.903
14	3.872	3.842	3.812	3.782	3.753	3.724	3.695	3.667	3.639	3.612
15	3.584	3.558	3.531	3.505	3.479	3.454	3.428	3.404	3.379	3.355
16	3.331	3.307	3.283	3.260	3.237	3.215	3.192	3.170	3.148	3.127
17	3.105	3.084	3.063	3.042	3.022	3.001	2.981	2.961	2.942	2.922
18	2.903	2.884	2.865	2.847	2.828	2.810	2.792	2.774	2.756	2.738
19	2.721	2.704	2.687	2.670	2.653	2.636	2.620	2.604	2.588	2.572
20	2.556	2.540	2.524	2.509	2.494	2.479	2.464	2.449	2.434	2.419
21	2.405	2.391	2.376	2.362	2.348	2.334	2.321	2.307	2.294	2.280
22	2.267	2.254	2.241	2.228	2.215	2.202	2.189	2.177	2.164	2.152
23	2.140	2.128	2.115	2.105	2.092	2.080	2.068	2.056	2.045	2.033
24	2.022	2.011	2.000	1.989	1.978	1.967	1.956	1.945	1.934	1.924
25	1.913	1.903	1.892	1.882	1.872	1.861	1.851	1.841	1.831	1.821
26	1.812	1.802	1.792	1.782	1.773	1.763	1.754	1.744	1.735	1.726
27	1.717	1.708	1.698	1.689	1.681	1.672	1.663	1.654	1.645	1.637
28	1.628	1.619	1.611	1.602	1.594	1.586	1.577	1.569	1.561	1.553
29	1.545	1.537	1.529	1.521	1.513	1.505	1.497	1.489	1.482	1.474
30	1.466	1.459	1.451	1.444	1.436	1.429	1.421	1.414	1.407	1.399
31	1.392	1.385	1.378	1.371	1.364	1.357	1.350	1.343	1.336	1.329
32	1.322	1.316	1.309	1.302	1.296	1.289	1.282	1.276	1.269	1.263
33	1.256	1.250	1.244	1.237	1.231	1.225	1.218	1.212	1.206	1.200
34	1.194	1.188	1.182	1.175	1.169	1.164	1.158	1.152	1.146	1.140
35	1.134	1.128	1.123	1.117	1.111	1.106	1.100	1.094	1.089	1.083
36	1.078	1.072	1.067	1.061	1.056	1.050	1.045	1.040	1.034	1.029
37	1.024	1.019	1.013	1.008	1.003	0.998	0.993	0.988	0.983	0.977
38	0.972	0.967	0.962	0.958	0.953	0.948	0.943	0.938	0.933	0.928
39	0.923	0.919	0.914	0.909	0.905	0.900	0.895	0.891	0.886	0.881
40	0.877	0.872	0.868	0.863	0.859	0.854	0.850	0.845	0.841	0.836
41	0.832	0.828	0.823	0.819	0.815	0.810	0.806	0.802	0.798	0.794
42	0.789	0.785	0.781	0.777	0.773	0.769	0.765	0.761	0.757	0.753
43	0.748	0.745	0.741	0.737	0.733	0.729	0.725	0.721	0.717	0.713
44	0.709	0.706	0.702	0.698	0.694	0.690	0.687	0.683	0.679	0.676
45	0.672	0.668	0.665	0.661	0.657	0.654	0.650	0.647	0.643	0.639
46	0.636	0.632	0.629	0.625	0.622	0.619	0.615	0.612	0.608	0.605
47	0.601	0.598	0.595	0.591	0.588	0.585	0.582	0.578	0.575	0.572
48	0.568	0.565	0.562	0.559	0.556	0.552	0.549	0.546	0.543	0.540
49	0.537	0.534	0.531	0.528	0.524	0.522	0.518	0.515	0.512	0.509

TABLE 4.7.4A (continued)

$$\frac{1}{2} \left(\frac{\cos^2 \theta}{\sin \theta} + \frac{\cos^2 \theta}{\theta} \right)$$

θ°	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
50	0.506	0.503	0.500	0.498	0.495	0.492	0.489	0.486	0.483	0.480
51	0.477	0.474	0.472	0.469	0.466	0.463	0.460	0.458	0.455	0.452
52	0.449	0.447	0.444	0.441	0.438	0.436	0.433	0.430	0.428	0.425
53	0.423	0.420	0.417	0.415	0.412	0.410	0.407	0.404	0.402	0.399
54	0.397	0.394	0.392	0.389	0.387	0.384	0.382	0.379	0.377	0.375
55	0.372	0.370	0.367	0.365	0.363	0.360	0.358	0.356	0.353	0.351
56	0.349	0.346	0.344	0.342	0.339	0.337	0.335	0.333	0.330	0.328
57	0.326	0.324	0.322	0.319	0.317	0.315	0.313	0.311	0.309	0.306
58	0.304	0.302	0.300	0.298	0.296	0.294	0.292	0.290	0.288	0.286
59	0.284	0.282	0.279	0.277	0.275	0.274	0.272	0.270	0.268	0.266
60	0.264	0.262	0.260	0.258	0.256	0.254	0.252	0.250	0.248	0.247
61	0.245	0.243	0.241	0.239	0.237	0.236	0.234	0.232	0.230	0.228
62	0.227	0.225	0.223	0.221	0.220	0.218	0.216	0.214	0.213	0.211
63	0.209	0.208	0.206	0.204	0.203	0.201	0.199	0.198	0.196	0.195
64	0.193	0.191	0.190	0.188	0.187	0.185	0.183	0.182	0.180	0.179
65	0.177	0.176	0.174	0.173	0.171	0.170	0.168	0.167	0.165	0.164
66	0.162	0.161	0.159	0.158	0.157	0.155	0.154	0.152	0.151	0.150
67	0.148	0.147	0.145	0.144	0.143	0.141	0.140	0.139	0.137	0.136
68	0.135	0.133	0.132	0.131	0.130	0.128	0.127	0.126	0.125	0.123
69	0.122	0.121	0.120	0.118	0.117	0.116	0.115	0.114	0.112	0.111
70	0.110	0.109	0.108	0.107	0.106	0.104	0.103	0.102	0.101	0.100
71	0.099	0.098	0.097	0.096	0.094	0.093	0.092	0.091	0.090	0.089
72	0.088	0.087	0.086	0.085	0.084	0.083	0.082	0.081	0.080	0.079
73	0.078	0.077	0.076	0.075	0.074	0.074	0.073	0.072	0.071	0.070
74	0.069	0.068	0.067	0.066	0.065	0.065	0.064	0.063	0.062	0.061
75	0.060	0.059	0.059	0.058	0.057	0.056	0.055	0.055	0.054	0.053
76	0.052	0.051	0.051	0.050	0.049	0.048	0.048	0.047	0.046	0.046
77	0.045	0.044	0.043	0.043	0.042	0.041	0.041	0.040	0.039	0.039
78	0.038	0.037	0.037	0.036	0.035	0.035	0.034	0.034	0.033	0.032
79	0.032	0.031	0.031	0.030	0.029	0.029	0.028	0.028	0.027	0.027
80	0.026	0.026	0.025	0.025	0.024	0.024	0.023	0.023	0.022	0.022
81	0.021	0.021	0.020	0.020	0.019	0.019	0.018	0.018	0.017	0.017
82	0.017	0.016	0.016	0.015	0.015	0.015	0.014	0.014	0.013	0.013
83	0.013	0.012	0.012	0.012	0.011	0.011	0.011	0.010	0.010	0.010
84	0.009	0.009	0.009	0.008	0.008	0.008	0.007	0.007	0.007	0.007
85	0.006	0.006	0.006	0.006	0.005	0.005	0.005	0.005	0.004	0.004
86	0.004	0.004	0.004	0.003	0.003	0.003	0.003	0.003	0.003	0.002
87	0.002	0.002	0.002	0.002	0.002	0.002	0.001	0.001	0.001	0.001
88	0.001	0.001	0.001	0.001	0.001	0.001	0.000	0.000	0.000	0.000

4.7. PRECISION MEASUREMENT OF LATTICE PARAMETERS OF POLYCRYSTALLINE SPECIMENS

TABLE 4.7.4B

 $\sin^2 \theta$ (read down) and $\cos^2 \theta$ (read up)

θ°	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	(+1.0)		Differences				
													.01	.02	.03	.04	.05
0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001	0.0001	0.0002	0.0002	0.0003	89	Interpolate				
1	.0003	.0004	.0004	.0005	.0006	.0007	.0008	.0009	.0010	.0011	.0012	88					
2	.0012	.0013	.0015	.0016	.0018	.0019	.0021	.0022	.0024	.0026	.0027	87					
3	.0027	.0029	.0031	.0033	.0035	.0037	.0039	.0042	.0044	.0046	.0049	86					
4	.0049	.0051	.0054	.0056	.0059	.0062	.0064	.0067	.0070	.0073	.0076	85					
5	.0076	.0079	.0082	.0085	.0089	.0092	.0095	.0099	.0102	.0106	.0109	84					
6	.0109	.0113	.0117	.0120	.0124	.0128	.0132	.0136	.0140	.0144	.0149	83					
7	.0149	.0153	.0157	.0161	.0166	.0170	.0175	.0180	.0184	.0189	.0194	82					
8	.0194	.0199	.0203	.0208	.0213	.0218	.0224	.0229	.0234	.0239	.0245	81					
9	.0245	.0250	.0256	.0261	.0267	.0272	.0278	.0284	.0290	.0296	.0302	80					
10	.0302	.0308	.0314	.0320	.0326	.0332	.0338	.0345	.0351	.0358	.0364	79	1	1	2	2	3
11	.0364	.0371	.0377	.0384	.0391	.0397	.0404	.0411	.0418	.0425	.0432	78	1	1	2	3	3
12	.0432	.0439	.0447	.0454	.0461	.0468	.0476	.0483	.0491	.0498	.0506	77	1	1	2	3	4
13	.0506	.0514	.0521	.0529	.0537	.0545	.0553	.0561	.0569	.0577	.0585	76	1	2	2	3	4
14	.0585	.0593	.0602	.0610	.0618	.0627	.0635	.0644	.0653	.0661	.0670	75	1	2	3	3	4
15	.0670	.0679	.0687	.0696	.0705	.0714	.0723	.0732	.0741	.0751	.0760	74	1	2	3	4	4
16	.0760	.0769	.0778	.0788	.0797	.0807	.0816	.0826	.0835	.0845	.0855	73	1	2	3	4	5
17	.0855	.0865	.0874	.0884	.0894	.0904	.0914	.0924	.0934	.0945	.0955	72	1	2	3	4	5
18	.0955	.0965	.0976	.0986	.0996	.1007	.1017	.1028	.1039	.1049	.1060	71	1	2	3	4	5
19	.1060	.1071	.1082	.1092	.1103	.1114	.1125	.1136	.1147	.1159	.1170	70	1	2	3	4	6
20	.1170	.1181	.1192	.1204	.1215	.1226	.1238	.1249	.1261	.1273	.1284	69	1	2	3	5	6
21	.1284	.1296	.1308	.1320	.1331	.1343	.1355	.1367	.1379	.1391	.1403	68	1	2	4	5	6
22	.1403	.1415	.1428	.1440	.1452	.1464	.1477	.1489	.1502	.1514	.1527	67	1	2	4	5	6
23	.1527	.1539	.1552	.1565	.1577	.1590	.1603	.1616	.1628	.1641	.1654	66	1	3	4	5	6
24	.1654	.1667	.1680	.1693	.1707	.1720	.1733	.1746	.1759	.1773	.1786	65	1	3	4	5	7
25	.1786	.1799	.1813	.1826	.1840	.1853	.1867	.1881	.1894	.1908	.1922	64	1	3	4	5	7
26	.1922	.1935	.1949	.1963	.1977	.1991	.2005	.2019	.2033	.2047	.2061	63	1	3	4	6	7
27	.2061	.2075	.2089	.2104	.2118	.2132	.2146	.2161	.2175	.2190	.2204	62	1	3	4	6	7
28	.2204	.2219	.2233	.2248	.2262	.2277	.2291	.2306	.2321	.2336	.2350	61	1	3	4	6	7
29	.2350	.2365	.2380	.2395	.2410	.2425	.2440	.2455	.2470	.2485	.2500	60	2	3	5	6	8
30	.2500	.2515	.2530	.2545	.2561	.2576	.2591	.2607	.2622	.2637	.2653	59	2	3	5	6	8
31	.2653	.2668	.2684	.2699	.2715	.2730	.2746	.2761	.2777	.2792	.2808	58	2	3	5	6	8
32	.2808	.2824	.2840	.2855	.2871	.2887	.2903	.2919	.2934	.2950	.2966	57	2	3	5	6	8
33	.2966	.2982	.2998	.3014	.3030	.3046	.3062	.3079	.3095	.3111	.3127	56	2	3	5	6	8
34	.3127	.3143	.3159	.3176	.3192	.3208	.3224	.3241	.3257	.3274	.3290	55	2	3	5	7	8
35	.3290	.3306	.3323	.3339	.3356	.3372	.3389	.3405	.3422	.3438	.3455	54	2	3	5	7	8
36	.3455	.3472	.3488	.3505	.3521	.3538	.3555	.3572	.3588	.3605	.3622	53	2	3	5	7	8
37	.3622	.3639	.3655	.3672	.3689	.3706	.3723	.3740	.3757	.3773	.3790	52	2	3	5	7	8
38	.3790	.3807	.3824	.3841	.3858	.3875	.3892	.3909	.3926	.3943	.3960	51	2	3	5	7	8
39	.3960	.3978	.3995	.4012	.4029	.4046	.4063	.4080	.4097	.4115	.4132	50	2	3	5	7	9
40	.4132	.4149	.4166	.4183	.4201	.4218	.4235	.4252	.4270	.4287	.4304	49	2	3	5	7	9
41	.4304	.4321	.4339	.4356	.4373	.4391	.4408	.4425	.4443	.4460	.4477	48	2	3	5	7	9
42	.4477	.4495	.4512	.4529	.4547	.4564	.4582	.4599	.4616	.4634	.4651	47	2	3	5	7	9
43	.4651	.4669	.4686	.4703	.4721	.4738	.4756	.4773	.4791	.4808	.4826	46	2	3	5	7	9
44	.4826	.4843	.4860	.4878	.4895	.4913	.4930	.4948	.4965	.4983	.5000	45	2	3	5	7	9
	(+1.0)	0.9	0.8	0.7	0.6	0.5	0.4	0.3	0.2	0.1	0.0	θ°					

 $\cos^2 \theta$ (read up)

4.7. PRECISION MEASUREMENT OF LATTICE PARAMETERS OF POLYCRYSTALLINE SPECIMENS

TABLE 4.7.4B (continued)
 $\sin^2 \theta$ (read down) and $\cos^2 \theta$ (read up)

θ°													Differences				
	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	(+1.0)		.01	.02	.03	.04	.05
45	0.5000	0.5017	0.5035	0.5052	0.5070	0.5087	0.5105	0.5122	0.5140	0.5157	0.5174	44	2	3	5	7	9
46	.5174	.5192	.5209	.5227	.5244	.5262	.5279	.5297	.5314	.5331	.5349	43	2	3	5	7	9
47	.5349	.5366	.5384	.5401	.5418	.5436	.5453	.5471	.5488	.5505	.5523	42	2	3	5	7	9
48	.5523	.5540	.5557	.5575	.5592	.5609	.5627	.5644	.5661	.5679	.5696	41	2	3	5	7	9
49	.5696	.5713	.5730	.5748	.5765	.5782	.5799	.5817	.5834	.5851	.5868	40	2	3	5	7	9
50	.5868	.5885	.5903	.5920	.5937	.5954	.5971	.5988	.6005	.6022	.6040	39	2	3	5	7	9
51	.6040	.6057	.6074	.6091	.6108	.6125	.6142	.6159	.6176	.6193	.6210	38	2	3	5	7	9
52	.6210	.6227	.6243	.6260	.6277	.6294	.6311	.6328	.6345	.6361	.6378	37	2	3	5	7	8
53	.6378	.6395	.6412	.6428	.6445	.6462	.6479	.6495	.6512	.6528	.6545	36	2	3	5	7	8
54	.6545	.6562	.6578	.6595	.6611	.6628	.6644	.6661	.6677	.6694	.6710	35	2	3	5	7	8
55	.6710	.6726	.6743	.6759	.6776	.6792	.6808	.6824	.6841	.6857	.6873	34	2	3	5	7	7
56	.6873	.6889	.6905	.6921	.6938	.6954	.6970	.6986	.7002	.7018	.7034	33	2	3	5	7	8
57	.7034	.7050	.7066	.7081	.7097	.7113	.7129	.7145	.7160	.7176	.7192	32	2	3	5	6	8
58	.7192	.7208	.7223	.7239	.7254	.7270	.7285	.7301	.7316	.7332	.7347	31	2	3	5	6	8
59	.7347	.7363	.7378	.7393	.7409	.7424	.7439	.7455	.7470	.7485	.7500	30	2	3	5	6	8
60	.7500	.7515	.7530	.7545	.7560	.7575	.7590	.7605	.7620	.7635	.7650	29	2	3	5	6	8
61	.7650	.7664	.7679	.7694	.7709	.7723	.7738	.7752	.7767	.7781	.7796	28	2	3	5	6	8
62	.7796	.7810	.7825	.7839	.7854	.7868	.7882	.7896	.7911	.7925	.7939	27	1	3	4	6	7
63	.7939	.7953	.7967	.7981	.7995	.8009	.8023	.8037	.8051	.8065	.8078	26	1	3	4	6	7
64	.8078	.8092	.8106	.8119	.8133	.8147	.8160	.8174	.8187	.8201	.8214	25	1	3	4	6	7
65	.8214	.8227	.8241	.8254	.8267	.8280	.8293	.8307	.8320	.8333	.8346	24	1	3	4	5	7
66	.8346	.8359	.8372	.8384	.8397	.8410	.8423	.8435	.8448	.8461	.8473	23	1	3	4	5	7
67	.8473	.8486	.8498	.8511	.8523	.8536	.8548	.8560	.8572	.8585	.8597	22	1	3	4	5	6
68	.8597	.8609	.8621	.8633	.8645	.8657	.8669	.8680	.8692	.8704	.8716	21	1	2	4	5	6
69	.8716	.8727	.8739	.8751	.8762	.8774	.8785	.8796	.8808	.8819	.8830	20	1	2	4	5	6
70	.8830	.8841	.8853	.8864	.8875	.8886	.8897	.8908	.8918	.8929	.8940	19	1	2	3	5	6
71	.8940	.8951	.8961	.8972	.8983	.8993	.9004	.9014	.9024	.9035	.9045	18	1	2	3	4	6
72	.9045	.9055	.9066	.9076	.9086	.9096	.9106	.9116	.9126	.9135	.9145	17	1	2	3	4	5
73	.9145	.9155	.9165	.9174	.9184	.9193	.9203	.9212	.9222	.9231	.9240	16	1	2	3	4	5
74	.9240	.9249	.9259	.9268	.9277	.9286	.9295	.9304	.9313	.9321	.9330	15	1	2	3	4	5
75	.9330	.9339	.9347	.9356	.9365	.9373	.9382	.9390	.9398	.9407	.9415	14	1	2	3	4	4
76	.9415	.9423	.9431	.9439	.9447	.9455	.9463	.9471	.9479	.9486	.9494	13	1	2	3	3	4
77	.9494	.9502	.9509	.9517	.9524	.9532	.9539	.9546	.9553	.9561	.9568	12	1	2	2	3	4
78	.9568	.9575	.9582	.9589	.9596	.9603	.9609	.9616	.9623	.9629	.9636	11	1	1	2	3	4
79	.9636	.9642	.9649	.9655	.9662	.9668	.9674	.9680	.9686	.9692	.9698	10	1	1	2	3	3
80	.9698	.9704	.9710	.9716	.9722	.9728	.9733	.9739	.9744	.9750	.9755	9	1	1	2	2	3
81	.9755	.9761	.9766	.9771	.9776	.9782	.9787	.9792	.9797	.9801	.9806	8					
82	.9806	.9811	.9816	.9820	.9825	.9830	.9834	.9839	.9843	.9847	.9851	7					
83	.9851	.9856	.9860	.9864	.9868	.9872	.9876	.9880	.9883	.9887	.9891	6					
84	.9891	.9894	.9898	.9901	.9905	.9908	.9911	.9915	.9918	.9921	.9924	5	Interpolate				
85	.9924	.9927	.9930	.9933	.9936	.9938	.9941	.9944	.9946	.9949	.9951	4					
86	.9951	.9954	.9956	.9958	.9961	.9963	.9965	.9967	.9969	.9971	.9973	3					
87	.9973	.9974	.9976	.9978	.9979	.9981	.9982	.9984	.9985	.9987	.9988	2					
88	.9988	.9989	.9990	.9991	.9992	.9993	.9994	.9995	.9996	.9996	.9997	1					
89	.9997	.9998	.9998	.9999	.9999	.9999	1.0000	1.0000	1.0000	1.0000	1.0000	0					
	(+1.0)	0.9	0.8	0.7	0.6	0.5	0.4	0.3	0.2	0.1	0.0	θ°					

 $\cos^2 \theta$ (read up)

TABLE 4.7.4C

 $\phi \tan \phi^\dagger$

ϕ°	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
0	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001	0.0001	0.0001	0.0002	0.0002
1	.0003	.0004	.0004	.0005	.0006	.0007	.0008	.0009	.0010	.0011
2	.0012	.0013	.0015	.0016	.0018	.0019	.0021	.0022	.0024	.0026
3	.0027	.0029	.0031	.0033	.0035	.0037	.0040	.0042	.0044	.0046
4	.0049	.0051	.0054	.0056	.0059	.0062	.0065	.0067	.0070	.0073
5	.0076	.0079	.0083	.0086	.0089	.0092	.0096	.0099	.0103	.0106
6	.0110	.0114	.0118	.0121	.0125	.0129	.0133	.0137	.0142	.0146
7	.0150	.0154	.0159	.0163	.0168	.0172	.0177	.0182	.0186	.0191
8	.0196	.0201	.0206	.0211	.0216	.0222	.0227	.0232	.0238	.0243
9	.0249	.0254	.0260	.0266	.0272	.0277	.0283	.0289	.0295	.0302
10	.0308	.0314	.0320	.0327	.0333	.0340	.0346	.0353	.0360	.0366
11	.0373	.0380	.0387	.0394	.0401	.0408	.0416	.0423	.0430	.0438
12	.0445	.0453	.0460	.0468	.0476	.0484	.0492	.0500	.0508	.0516
13	.0524	.0532	.0540	.0549	.0557	.0566	.0574	.0583	.0592	.0600
14	.0609	.0618	.0627	.0636	.0645	.0654	.0664	.0673	.0682	.0692
15	.0701	.0711	.0721	.0731	.0740	.0750	.0760	.0770	.0780	.0791
16	.0801	.0811	.0821	.0832	.0842	.0853	.0864	.0874	.0885	.0896
17	.0907	.0918	.0929	.0940	.0952	.0963	.0974	.0986	.0997	.1009
18	.1021	.1033	.1044	.1056	.1068	.1080	.1093	.1105	.1117	.1129
19	.1142	.1154	.1167	.1180	.1192	.1205	.1218	.1231	.1244	.1257
20	.1270	.1284	.1297	.1311	.1324	.1338	.1351	.1365	.1379	.1393
21	.1407	.1421	.1435	.1449	.1464	.1478	.1493	.1507	.1522	.1537
22	.1551	.1566	.1581	.1596	.1611	.1627	.1642	.1657	.1673	.1688
23	.1704	.1720	.1735	.1751	.1767	.1783	.1800	.1816	.1832	.1848
24	.1865	.1882	.1898	.1915	.1932	.1949	.1966	.1983	.2000	.2017
25	.2035	.2052	.2070	.2087	.2105	.2123	.2141	.2159	.2177	.2195
26	.2213	.2232	.2250	.2269	.2287	.2306	.2325	.2344	.2363	.2382
27	.2401	.2420	.2440	.2459	.2479	.2499	.2518	.2538	.2558	.2578
28	.2598	.2619	.2639	.2660	.2680	.2701	.2722	.2742	.2763	.2784
29	.2806	.2827	.2848	.2870	.2891	.2913	.2935	.2957	.2979	.3001
30	.3023	.3045	.3068	.3090	.3113	.3136	.3158	.3181	.3205	.3228
31	.3251	.3274	.3298	.3321	.3345	.3369	.3393	.3417	.3441	.3466
32	.3490	.3514	.3539	.3564	.3589	.3614	.3639	.3664	.3689	.3715
33	.3740	.3766	.3792	.3818	.3844	.3870	.3896	.3923	.3949	.3976
34	.4003	.4030	.4057	.4084	.4111	.4138	.4166	.4194	.4221	.4249
35	.4277	.4306	.4334	.4362	.4391	.4420	.4448	.4477	.4506	.4536
36	.4565	.4595	.4624	.4654	.4684	.4714	.4744	.4774	.4805	.4835
37	.4866	.4897	.4928	.4959	.4991	.5022	.5054	.5086	.5117	.5149
38	.5182	.5214	.5247	.5279	.5312	.5345	.5378	.5411	.5445	.5478
39	.5512	.5546	.5580	.5614	.5649	.5683	.5718	.5753	.5788	.5823
40	.5858	.5894	.5929	.5965	.6001	.6037	.6073	.6110	.6147	.6183
41	.6220	.6258	.6295	.6333	.6370	.6408	.6446	.6484	.6523	.6562
42	.6600	.6639	.6678	.6718	.6757	.6797	.6837	.6877	.6917	.6958
43	.6998	.7039	.7080	.7122	.7163	.7205	.7247	.7289	.7331	.7373
44	.7416	.7459	.7502	.7545	.7589	.7632	.7676	.7720	.7765	.7809
45	.7854	.7899	.7944	.7990	.8035	.8081	.8127	.8173	.8220	.8267

 \dagger Calculated by Marian Mack and Jeanne Taylor.

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Section 5

PHYSICS OF DIFFRACTION METHODS

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in collaboration with

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W. COCHRAN (Lorentz-polarization corrections)

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R. A. L. SULLIVAN (Revision of Tables 5.2.5E, F, G)

	PAGE
5.1. BASIC DEFINITIONS AND FORMULAE	237
5.2. INTENSITY OF RADIATION DIFFRACTED BY A CRYSTAL	241
5.3. ABSORPTION CORRECTIONS	291
5.4. MOSAIC THEORY	313
5.5. SUMMARY OF FORMULAE FOR INTEGRATED INTENSITIES	314

5.1. Basic Definitions and Formulae

5.1.1. Definitions of Symbols

I_0 : Energy of X-radiation falling normally on unit area per second.
 I : Total energy of radiation per second in a limited X-ray beam.
 e, m : Electronic charge and mass.
 λ : Wavelength of X-rays.
 c : Velocity of light.
 h : Planck's constant.
 k : Boltzmann's constant.
 μ : Linear absorption coefficient.
 2θ : Angle between incident and diffracted beams.
 a, b, c : Lengths of edges of unit cell.
 V : Volume of crystal, or of irradiated part of a powder sample.
 V_c : Volume of unit cell.
 N : Number of unit cells per unit volume.
 x_r, y_r, z_r : Co-ordinates of an atom r , expressed as fractions of a, b and c .
 hkl : Indices of diffraction.
 f_0 : Atomic scattering factor for atom at rest.
 $F(hkl)$: Structure factor, for the unit cell, of the order of diffraction hkl .
 $|F(hkl)|$: Modulus of the structure factor—the structure amplitude.
 A : Transmission factor.
 A^* : Absorption factor.
 ρ : Integrated reflection from crystal element.
 ρ' : Integrated reflection from extended crystal face.
 L : Lorentz factor.
 p : Polarization factor.
 p' : Multiplicity factor for single crystal methods.
 p'' : Multiplicity factor for powder method.

5.1.2. Formulae for Scattering by an Electron

Under the influence of a polarized wave of unit amplitude, an electron scatters a coherent wave which has an amplitude, at a distance r , of

$$\frac{e^2}{rmc^2} \quad \dots (1)$$

if the electric vector is perpendicular to the plane containing the incident and scattered beams. If the electric vector is parallel to the plane of the incident and scattered beams, the amplitude of the scattered radiation is

$$\frac{e^2}{rmc^2} \cos 2\theta \quad \dots (2)$$

If the radiation is unpolarized, with unit mean amplitude, the mean amplitude of the scattered wave is

$$\frac{e^2}{rmc^2} \left\{ \frac{1 + \cos^2 2\theta}{2} \right\}^{\frac{1}{2}} \quad \dots (3)$$

The function $(1 + \cos^2 2\theta)/2$ is tabulated in Table 5.1.2.

5.1.3. Formula for the Atomic Scattering Factor f_0

An atom contains electrons distributed over a finite region in space; for any given scattering direction, the electrons at different points contribute waves with different paths and consequently different phases, and thus the total scattering by an atom depends upon the distribution of electrons within it. If $U(r)dr$ is the number of electrons lying between the distances r and $r+dr$ from the centre, and the electron distribution is spherically symmetrical, the atom will scatter at any particular angle 2θ as though it were equivalent to f_0 electrons, where

$$f_0 = \int_0^\infty \frac{U(r) \sin (4\pi r \sin \theta / \lambda)}{4\pi r \sin \theta / \lambda} dr \quad \dots (4)$$

At very small values of θ , f_0 approximates to Z , the atomic number.

Consult 2.5.3.2(a) (page 70) and 6.3.3 (page 323) for expressions for f_0 when the electron distribution is not spherically symmetrical.

5.1. BASIC DEFINITIONS AND FORMULAE

TABLE 5.1.2

Polarization Factor, $p = \frac{1 + \cos^2 2\theta}{2}$, as a Function of $\sin \theta$

$\sin \theta$	0.000	0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009
0.00	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	0.9999	0.9999	0.9999	0.9998
0.01	0.9998	0.9998	0.9997	0.9997	0.9996	0.9996	0.9995	0.9994	0.9994	0.9993
0.02	0.9992	0.9991	0.9990	0.9989	0.9988	0.9988	0.9986	0.9985	0.9984	0.9983
0.03	0.9982	0.9981	0.9980	0.9978	0.9977	0.9976	0.9974	0.9973	0.9971	0.9970
0.04	0.9968	0.9966	0.9965	0.9963	0.9961	0.9960	0.9958	0.9956	0.9954	0.9952
0.05	0.9950	0.9948	0.9946	0.9944	0.9942	0.9940	0.9937	0.9935	0.9933	0.9931
0.06	0.9928	0.9926	0.9923	0.9921	0.9918	0.9916	0.9913	0.9911	0.9908	0.9905
0.07	0.9902	0.9900	0.9897	0.9894	0.9891	0.9888	0.9885	0.9882	0.9879	0.9876
0.08	0.9873	0.9870	0.9866	0.9863	0.9860	0.9857	0.9853	0.9850	0.9846	0.9843
0.09	0.9839	0.9836	0.9832	0.9829	0.9825	0.9821	0.9817	0.9814	0.9810	0.9806
0.10	0.9802	0.9798	0.9794	0.9790	0.9786	0.9782	0.9778	0.9774	0.9769	0.9765
0.11	0.9761	0.9757	0.9752	0.9748	0.9743	0.9739	0.9735	0.9730	0.9725	0.9721
0.12	0.9716	0.9711	0.9707	0.9702	0.9697	0.9692	0.9688	0.9683	0.9678	0.9673
0.13	0.9668	0.9663	0.9658	0.9652	0.9647	0.9642	0.9637	0.9632	0.9626	0.9621
0.14	0.9616	0.9610	0.9605	0.9599	0.9594	0.9588	0.9583	0.9577	0.9572	0.9566
0.15	0.9560	0.9554	0.9549	0.9543	0.9537	0.9531	0.9525	0.9519	0.9513	0.9507
0.16	0.9501	0.9495	0.9489	0.9483	0.9477	0.9470	0.9464	0.9458	0.9451	0.9445
0.17	0.9439	0.9432	0.9426	0.9419	0.9413	0.9406	0.9400	0.9393	0.9386	0.9380
0.18	0.9373	0.9366	0.9359	0.9353	0.9346	0.9339	0.9332	0.9325	0.9318	0.9311
0.19	0.9304	0.9297	0.9290	0.9283	0.9276	0.9268	0.9261	0.9254	0.9247	0.9239
0.20	0.9232	0.9225	0.9217	0.9210	0.9202	0.9195	0.9187	0.9180	0.9172	0.9165
0.21	0.9157	0.9149	0.9142	0.9134	0.9126	0.9118	0.9110	0.9103	0.9095	0.9087
0.22	0.9079	0.9071	0.9063	0.9055	0.9047	0.9039	0.9031	0.9023	0.9014	0.9006
0.23	0.8998	0.8990	0.8981	0.8973	0.8965	0.8956	0.8948	0.8940	0.8931	0.8923
0.24	0.8914	0.8906	0.8897	0.8889	0.8880	0.8872	0.8863	0.8854	0.8846	0.8837
0.25	0.8828	0.8819	0.8811	0.8802	0.8793	0.8784	0.8775	0.8766	0.8757	0.8748
0.26	0.8739	0.8730	0.8721	0.8712	0.8703	0.8694	0.8685	0.8676	0.8667	0.8658
0.27	0.8648	0.8639	0.8630	0.8621	0.8611	0.8602	0.8593	0.8583	0.8574	0.8564
0.28	0.8555	0.8545	0.8536	0.8527	0.8517	0.8507	0.8498	0.8488	0.8479	0.8469
0.29	0.8459	0.8450	0.8440	0.8430	0.8421	0.8411	0.8401	0.8391	0.8382	0.8372
0.30	0.8362	0.8352	0.8342	0.8332	0.8322	0.8313	0.8303	0.8293	0.8283	0.8273
0.31	0.8263	0.8253	0.8243	0.8233	0.8223	0.8212	0.8202	0.8192	0.8182	0.8172
0.32	0.8162	0.8152	0.8141	0.8131	0.8121	0.8111	0.8100	0.8090	0.8080	0.8070
0.33	0.8059	0.8049	0.8039	0.8028	0.8018	0.8007	0.7997	0.7987	0.7976	0.7966
0.34	0.7955	0.7945	0.7934	0.7924	0.7913	0.7903	0.7892	0.7882	0.7871	0.7861
0.35	0.7850	0.7840	0.7829	0.7818	0.7808	0.7797	0.7787	0.7776	0.7765	0.7755
0.36	0.7744	0.7733	0.7723	0.7712	0.7701	0.7690	0.7680	0.7669	0.7658	0.7648
0.37	0.7637	0.7626	0.7615	0.7605	0.7594	0.7583	0.7572	0.7561	0.7551	0.7540
0.38	0.7529	0.7518	0.7507	0.7497	0.7486	0.7475	0.7464	0.7453	0.7442	0.7432
0.39	0.7421	0.7410	0.7399	0.7388	0.7377	0.7366	0.7356	0.7345	0.7334	0.7323

5.1. BASIC DEFINITIONS AND FORMULAE

TABLE 5.1.2 (continued)

Polarization Factor, $p = \frac{1 + \cos^2 2\theta}{2}$, as a Function of $\sin \theta$

$\sin \theta$	0.000	0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009
0.40	0.7312	0.7301	0.7290	0.7279	0.7268	0.7258	0.7247	0.7236	0.7225	0.7214
0.41	0.7203	0.7192	0.7181	0.7171	0.7160	0.7149	0.7138	0.7127	0.7116	0.7105
0.42	0.7094	0.7083	0.7073	0.7062	0.7051	0.7040	0.7029	0.7018	0.7007	0.6997
0.43	0.6986	0.6975	0.6964	0.6953	0.6942	0.6932	0.6921	0.6910	0.6899	0.6888
0.44	0.6878	0.6867	0.6856	0.6845	0.6835	0.6824	0.6813	0.6802	0.6792	0.6781
0.45	0.6770	0.6759	0.6749	0.6738	0.6727	0.6717	0.6706	0.6695	0.6685	0.6674
0.46	0.6663	0.6653	0.6642	0.6632	0.6621	0.6611	0.6600	0.6589	0.6579	0.6568
0.47	0.6558	0.6547	0.6537	0.6527	0.6516	0.6506	0.6495	0.6485	0.6474	0.6464
0.48	0.6454	0.6443	0.6433	0.6423	0.6412	0.6402	0.6392	0.6382	0.6371	0.6361
0.49	0.6351	0.6341	0.6331	0.6320	0.6310	0.6300	0.6290	0.6280	0.6270	0.6260
0.50	0.6250	0.6240	0.6230	0.6220	0.6210	0.6200	0.6190	0.6181	0.6171	0.6161
0.51	0.6151	0.6141	0.6132	0.6122	0.6112	0.6102	0.6093	0.6083	0.6073	0.6064
0.52	0.6054	0.6045	0.6035	0.6026	0.6016	0.6007	0.5997	0.5988	0.5979	0.5969
0.53	0.5960	0.5951	0.5942	0.5932	0.5923	0.5914	0.5905	0.5896	0.5887	0.5878
0.54	0.5869	0.5860	0.5851	0.5842	0.5833	0.5824	0.5815	0.5806	0.5798	0.5789
0.55	0.5780	0.5771	0.5763	0.5754	0.5746	0.5737	0.5729	0.5720	0.5712	0.5703
0.56	0.5695	0.5687	0.5678	0.5670	0.5662	0.5654	0.5645	0.5637	0.5629	0.5621
0.57	0.5613	0.5605	0.5597	0.5589	0.5582	0.5574	0.5566	0.5558	0.5551	0.5543
0.58	0.5535	0.5528	0.5520	0.5513	0.5505	0.5498	0.5491	0.5483	0.5476	0.5469
0.59	0.5461	0.5454	0.5447	0.5440	0.5433	0.5426	0.5419	0.5412	0.5406	0.5399
0.60	0.5392	0.5385	0.5379	0.5372	0.5366	0.5359	0.5353	0.5346	0.5340	0.5333
0.61	0.5327	0.5321	0.5315	0.5309	0.5303	0.5297	0.5291	0.5285	0.5279	0.5273
0.62	0.5267	0.5262	0.5256	0.5250	0.5245	0.5239	0.5234	0.5228	0.5223	0.5218
0.63	0.5213	0.5207	0.5202	0.5197	0.5192	0.5187	0.5182	0.5178	0.5173	0.5168
0.64	0.5163	0.5159	0.5154	0.5150	0.5145	0.5141	0.5137	0.5132	0.5128	0.5124
0.65	0.5120	0.5116	0.5112	0.5108	0.5105	0.5101	0.5097	0.5093	0.5090	0.5086
0.66	0.5083	0.5080	0.5076	0.5073	0.5070	0.5067	0.5064	0.5061	0.5058	0.5055
0.67	0.5052	0.5050	0.5047	0.5044	0.5042	0.5039	0.5037	0.5035	0.5033	0.5030
0.68	0.5028	0.5026	0.5024	0.5022	0.5021	0.5019	0.5017	0.5016	0.5014	0.5013
0.69	0.5011	0.5010	0.5009	0.5008	0.5007	0.5006	0.5005	0.5004	0.5003	0.5003
0.70	0.5002	0.5001	0.5001	0.5001	0.5000	0.5000	0.5000	0.5000	0.5000	0.5000
0.71	0.5000	0.5001	0.5001	0.5001	0.5002	0.5003	0.5003	0.5004	0.5005	0.5006
0.72	0.5007	0.5008	0.5009	0.5010	0.5012	0.5013	0.5015	0.5016	0.5018	0.5020
0.73	0.5022	0.5024	0.5026	0.5028	0.5030	0.5032	0.5035	0.5037	0.5040	0.5043
0.74	0.5045	0.5048	0.5051	0.5054	0.5057	0.5061	0.5064	0.5067	0.5071	0.5074
0.75	0.5078	0.5082	0.5086	0.5090	0.5094	0.5098	0.5102	0.5107	0.5111	0.5116
0.76	0.5120	0.5125	0.5130	0.5135	0.5140	0.5145	0.5151	0.5156	0.5161	0.5167
0.77	0.5173	0.5178	0.5184	0.5190	0.5196	0.5202	0.5209	0.5215	0.5222	0.5228
0.78	0.5235	0.5242	0.5249	0.5256	0.5263	0.5270	0.5278	0.5285	0.5293	0.5300
0.79	0.5308	0.5316	0.5324	0.5332	0.5340	0.5349	0.5357	0.5366	0.5374	0.5383

5.1. BASIC DEFINITIONS AND FORMULAE

TABLE 5.1.2 (*continued*)Polarization Factor, $p = \frac{1 + \cos^2 2\theta}{2}$, as a Function of $\sin \theta$

$\sin \theta$	0.000	0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009
0.80	0.5392	0.5401	0.5410	0.5419	0.5429	0.5438	0.5448	0.5458	0.5467	0.5477
0.81	0.5487	0.5497	0.5508	0.5518	0.5529	0.5539	0.5550	0.5561	0.5572	0.5583
0.82	0.5594	0.5606	0.5617	0.5629	0.5641	0.5652	0.5664	0.5677	0.5689	0.5701
0.83	0.5714	0.5726	0.5739	0.5752	0.5765	0.5778	0.5791	0.5805	0.5818	0.5832
0.84	0.5845	0.5859	0.5873	0.5887	0.5902	0.5916	0.5931	0.5945	0.5960	0.5975
0.85	0.5990	0.6005	0.6021	0.6036	0.6052	0.6067	0.6083	0.6099	0.6115	0.6132
0.86	0.6148	0.6165	0.6181	0.6198	0.6215	0.6232	0.6250	0.6267	0.6284	0.6302
0.87	0.6320	0.6338	0.6356	0.6374	0.6393	0.6411	0.6430	0.6449	0.6468	0.6487
0.88	0.6506	0.6525	0.6545	0.6564	0.6584	0.6604	0.6624	0.6645	0.6665	0.6686
0.89	0.6706	0.6727	0.6748	0.6769	0.6791	0.6812	0.6834	0.6856	0.6878	0.6900
0.90	0.6922	0.6944	0.6967	0.6990	0.7012	0.7035	0.7059	0.7082	0.7105	0.7129
0.91	0.7153	0.7177	0.7201	0.7225	0.7250	0.7274	0.7299	0.7324	0.7349	0.7374
0.92	0.7400	0.7425	0.7451	0.7477	0.7503	0.7529	0.7556	0.7582	0.7609	0.7636
0.93	0.7663	0.7690	0.7718	0.7745	0.7773	0.7801	0.7829	0.7857	0.7886	0.7914
0.94	0.7943	0.7972	0.8001	0.8030	0.8060	0.8089	0.8119	0.8149	0.8179	0.8210
0.95	0.8240	0.8271	0.8302	0.8333	0.8364	0.8395	0.8427	0.8459	0.8490	0.8523
0.96	0.8555	0.8587	0.8620	0.8653	0.8686	0.8719	0.8752	0.8786	0.8820	0.8854
0.97	0.8888	0.8922	0.8957	0.8991	0.9026	0.9061	0.9096	0.9132	0.9167	0.9203
0.98	0.9239	0.9275	0.9312	0.9348	0.9385	0.9422	0.9459	0.9497	0.9534	0.9572
0.99	0.9610	0.9648	0.9686	0.9725	0.9763	0.9802	0.9841	0.9881	0.9920	0.9960

5.2. Intensity of Radiation Diffracted by a Crystal

5.2.1. Structure Factor

The unit cell of a crystal contains atoms in various positions, and the waves scattered in any order of diffraction hkl by the different atoms will have various phase differences with respect to each other. The amplitude of the resultant wave, when “atomic functions” (2.5.3.2(a), page 70) are used, is given by the expression

$$F(hkl) = \sum f_{0,r} \exp 2\pi i(hx_r + ky_r + lz_r) \dots (1)$$

where $f_{0,r}$ is the scattering factor of the r th atom. The modulus of $F(hkl)$ is known as the *structure amplitude*, and is the ratio of the amplitude of the wave scattered in the order hkl by the atoms in one unit cell to the amplitude of the wave scattered by a single electron under the same conditions. $|F(hkl)|$ is thus a pure number.

The ratio of the structure amplitude of a reflection to the maximum possible at the corresponding Bragg angle (that is, if all the atoms were scattering in phase) is called the *unitary structure amplitude*. The unitary structure amplitude of a reflection can be derived by dividing the observed structure amplitude by the sum of the scattering factors, at the corresponding angle, of the atoms in the unit cell.

The quantity $F(hkl)$ is known as the *structure factor*. Only its modulus can be observed experimentally. In general, $F(hkl)$ is a complex quantity (that is, the phase of the scattered wave may have *any* phase difference with respect to that of a wave scattered by an atom at the origin of the unit cell).

$$\text{Then } |F(hkl)|^2 = \{\sum f_{0,r} \cos 2\pi(hx_r + ky_r + lz_r)\}^2 + \{\sum f_{0,r} \sin 2\pi(hx_r + ky_r + lz_r)\}^2 \dots (2)$$

If, however, the crystal has a centre of symmetry, the structure factor is real and is given by the equation

$$F(hkl) = \sum f_{0,r} \cos 2\pi(hx_r + ky_r + lz_r) \dots (3)$$

This expression may be positive or negative (that is, the phase of the scattered wave is 0 or π with respect to the phase of a wave scattered by an atom at the origin).

For other symmetries, various other expressions for the structure factor arise; these are given in detail in Volume I.

5.2.2. Temperature Factor

The structure amplitudes calculated by means of equations 5.2.1 (1), (2) and (3) cannot be directly compared with observed values because the values of f_0 are computed for atoms at rest; normally, atoms in a crystal have movements due to temperature, so that at any instant corresponding atoms are not separated by exact multiples of the cell dimensions. Thus two such atoms will not scatter exactly in phase in any particular order, and the structure factor will be smaller than calculated. The effect can be allowed for by reducing

the scattering factor of each atom to $f = f_0 \exp(-M)$, where

$$M = 8\pi^2 \overline{u_s^2} \sin^2 \theta / \lambda^2 = 2\pi^2 \overline{u_s^2} / d^2 \dots (4)$$

$\overline{u_s^2}$ being the mean square displacement of the atoms, from their mean positions, in a direction perpendicular to the reflecting planes, interplanar spacing d (Debye [7] [8]).

This treatment is only approximate. Each atom should have its own value of M , which itself may be dependent upon the orientation of the reflecting planes. For much X-ray work, however, it is sufficient to assume that a mean value of M is appropriate; the structure-factor formula 5.2.1(1) then becomes

$$F(hkl) = \sum f_{0,r} \exp 2\pi i(hx_r + ky_r + lz_r) \exp(-M) \\ = \sum f_{0,r} \exp 2\pi i(hx_r + ky_r + lz_r) \exp(-B \sin^2 \theta / \lambda^2) \dots (5)$$

where B is a constant. The probability that B will vary from atom to atom, and with direction in the crystal, should always be borne in mind. The least-squares derivation of individual temperature factors is given in 6.4.1.2 (γ) (δ), page 327.

Values of $\exp(-B \sin^2 \theta / \lambda^2)$ to cover the range normally met with in practice are given in Table 5.2.2A.

The quantities $B = 8\pi^2 \overline{u_s^2}$ are not easily derived theoretically, as they depend in a complicated way upon temperature and upon the interatomic forces. Debye gives the expression

$$B = \frac{6h^2}{m_a k \Theta} \left\{ \frac{\phi(x)}{x} + \frac{1}{4} \right\} \dots (6)$$

where Θ is the characteristic temperature, m_a is the mass of the atoms or vibrating systems, x is the ratio of Θ to the absolute temperature, and

$$\phi(x) = \frac{1}{x} \int_0^x \frac{\xi}{e^\xi - 1} d\xi \dots (7)$$

Equation (6) is, however, strictly applicable only to cubic crystals containing one type of atom.

Values of $\phi(x)$ as a function of x are given in Table 5.2.2B.

Waller [15] and Waller and James [16] give an equation for $\overline{u_s^2}$:

$$\overline{u_s^2} = \beta T + \gamma T^{-1} + \delta T^{-3} + \dots \dots (8)$$

where T is the absolute temperature, $\gamma = h^2 / 48\pi^2 m_a k$, and β and δ are constants which depend upon the interatomic forces and cannot easily be derived, although for certain simple crystals β can be derived from the elastic constants, and

$$\delta = \frac{113}{288} \frac{\Theta^2}{\bar{A} n^2} 10^{-16} \dots (9)$$

In this equation \bar{A} is the mean atomic weight and n is the number of atoms per c.c.

(Continued on page 265)

TABLE 5.2.2A
exp $(-B \sin^2 \theta/\lambda^2)$

$\frac{\sin \theta}{\lambda}$	$B=0.1$	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
0.01	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.02	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.03	1.000	1.000	1.000	1.000	1.000	0.999	0.999	0.999	0.999	0.999
0.04	1.000	1.000	1.000	0.999	0.999	0.999	0.999	0.999	0.999	0.999
0.05	1.000	1.000	0.999	0.999	0.999	0.999	0.998	0.998	0.998	0.998
0.06	1.000	0.999	0.999	0.999	0.998	0.998	0.997	0.997	0.997	0.996
0.07	1.000	0.999	0.999	0.998	0.998	0.997	0.997	0.996	0.996	0.995
0.08	0.999	0.999	0.998	0.997	0.997	0.996	0.996	0.995	0.994	0.994
0.09	0.999	0.998	0.998	0.997	0.996	0.995	0.994	0.994	0.993	0.992
0.10	0.999	0.998	0.997	0.996	0.995	0.994	0.993	0.992	0.991	0.990
0.11	0.999	0.998	0.996	0.995	0.994	0.993	0.992	0.990	0.989	0.988
0.12	0.999	0.997	0.996	0.994	0.993	0.991	0.990	0.989	0.987	0.986
0.13	0.998	0.997	0.995	0.993	0.992	0.990	0.988	0.987	0.985	0.983
0.14	0.998	0.996	0.994	0.992	0.990	0.988	0.986	0.984	0.983	0.981
0.15	0.998	0.996	0.993	0.991	0.989	0.987	0.984	0.982	0.980	0.978
0.16	0.997	0.995	0.992	0.990	0.987	0.985	0.982	0.980	0.977	0.975
0.17	0.997	0.994	0.991	0.989	0.986	0.983	0.980	0.977	0.974	0.972
0.18	0.997	0.994	0.990	0.987	0.984	0.981	0.978	0.974	0.971	0.968
0.19	0.996	0.993	0.989	0.986	0.982	0.979	0.975	0.972	0.968	0.965
0.20	0.996	0.992	0.988	0.984	0.980	0.976	0.972	0.969	0.965	0.961
0.21	0.996	0.991	0.987	0.983	0.978	0.974	0.970	0.965	0.961	0.957
0.22	0.995	0.990	0.986	0.981	0.976	0.971	0.967	0.962	0.957	0.953
0.23	0.995	0.989	0.984	0.979	0.974	0.969	0.964	0.959	0.954	0.948
0.24	0.994	0.989	0.983	0.977	0.972	0.966	0.960	0.955	0.949	0.944
0.25	0.994	0.988	0.981	0.975	0.969	0.963	0.957	0.951	0.945	0.939
0.26	0.993	0.987	0.980	0.973	0.967	0.960	0.954	0.947	0.941	0.935
0.27	0.993	0.986	0.978	0.971	0.964	0.957	0.950	0.943	0.936	0.930
0.28	0.992	0.984	0.977	0.969	0.962	0.954	0.947	0.939	0.932	0.925
0.29	0.992	0.983	0.975	0.967	0.959	0.951	0.943	0.935	0.927	0.919
0.30	0.991	0.982	0.973	0.965	0.956	0.947	0.939	0.931	0.922	0.914
0.31	0.990	0.981	0.972	0.962	0.953	0.944	0.935	0.926	0.917	0.908
0.32	0.990	0.980	0.970	0.960	0.950	0.940	0.931	0.921	0.912	0.903
0.33	0.989	0.978	0.968	0.957	0.947	0.937	0.927	0.917	0.907	0.897
0.34	0.989	0.977	0.966	0.955	0.944	0.933	0.922	0.912	0.901	0.891
0.35	0.988	0.976	0.964	0.952	0.941	0.929	0.918	0.907	0.896	0.885
0.36	0.987	0.974	0.962	0.949	0.937	0.925	0.913	0.902	0.890	0.878
0.37	0.986	0.973	0.960	0.947	0.934	0.921	0.908	0.896	0.884	0.872
0.38	0.986	0.972	0.958	0.944	0.930	0.917	0.904	0.891	0.878	0.866
0.39	0.985	0.970	0.955	0.941	0.927	0.913	0.899	0.885	0.872	0.859
0.40	0.984	0.969	0.953	0.938	0.923	0.908	0.894	0.880	0.866	0.852
0.41	0.983	0.967	0.951	0.935	0.919	0.904	0.889	0.874	0.860	0.845
0.42	0.983	0.965	0.948	0.932	0.916	0.900	0.884	0.868	0.853	0.838
0.43	0.982	0.964	0.946	0.929	0.912	0.895	0.879	0.863	0.847	0.831
0.44	0.981	0.962	0.944	0.925	0.908	0.890	0.873	0.857	0.840	0.824
0.45	0.980	0.960	0.941	0.922	0.904	0.886	0.868	0.850	0.833	0.817
0.46	0.979	0.959	0.938	0.919	0.900	0.881	0.862	0.844	0.827	0.809
0.47	0.978	0.957	0.936	0.915	0.895	0.876	0.857	0.838	0.820	0.802
0.48	0.977	0.955	0.933	0.912	0.891	0.871	0.851	0.832	0.813	0.794
0.49	0.976	0.953	0.931	0.908	0.887	0.866	0.845	0.825	0.806	0.787
0.50	0.975	0.951	0.928	0.905	0.882	0.861	0.839	0.819	0.799	0.779

TABLE 5.2.2A (continued)

 $\exp(-B \sin^2 \theta / \lambda^2)$

$\frac{\sin \theta}{\lambda}$	$B=0.1$	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
0.51	0.974	0.949	0.925	0.901	0.878	0.856	0.834	0.812	0.791	0.771
0.52	0.973	0.947	0.922	0.897	0.874	0.850	0.828	0.805	0.784	0.763
0.53	0.972	0.945	0.919	0.894	0.869	0.845	0.821	0.799	0.777	0.755
0.54	0.971	0.943	0.916	0.890	0.864	0.839	0.815	0.792	0.769	0.747
0.55	0.970	0.941	0.913	0.886	0.860	0.834	0.809	0.785	0.762	0.739
0.56	0.969	0.939	0.910	0.882	0.855	0.828	0.803	0.778	0.754	0.731
0.57	0.968	0.937	0.907	0.878	0.850	0.823	0.797	0.771	0.746	0.723
0.58	0.967	0.935	0.904	0.874	0.845	0.817	0.790	0.764	0.739	0.714
0.59	0.966	0.933	0.901	0.870	0.840	0.812	0.784	0.757	0.731	0.706
0.60	0.965	0.931	0.898	0.866	0.835	0.806	0.777	0.750	0.723	0.698
0.61	0.963	0.928	0.894	0.862	0.830	0.800	0.771	0.743	0.715	0.689
0.62	0.962	0.926	0.891	0.857	0.825	0.794	0.764	0.735	0.708	0.681
0.63	0.961	0.924	0.888	0.853	0.820	0.788	0.757	0.728	0.700	0.672
0.64	0.960	0.921	0.884	0.849	0.815	0.782	0.751	0.721	0.692	0.664
0.65	0.959	0.919	0.881	0.845	0.810	0.776	0.744	0.713	0.684	0.655
0.66	0.957	0.917	0.877	0.840	0.804	0.770	0.737	0.706	0.676	0.647
0.67	0.956	0.914	0.874	0.836	0.799	0.764	0.730	0.698	0.668	0.638
0.68	0.955	0.912	0.870	0.831	0.794	0.758	0.723	0.691	0.660	0.630
0.69	0.954	0.909	0.867	0.827	0.788	0.752	0.717	0.683	0.651	0.621
0.70	0.952	0.907	0.863	0.822	0.783	0.745	0.710	0.676	0.643	0.613
0.71	0.951	0.904	0.860	0.817	0.777	0.739	0.703	0.668	0.635	0.604
0.72	0.949	0.902	0.856	0.813	0.772	0.733	0.696	0.661	0.627	0.595
0.73	0.948	0.899	0.852	0.808	0.766	0.726	0.689	0.653	0.619	0.587
0.74	0.947	0.896	0.849	0.803	0.760	0.720	0.682	0.645	0.611	0.578
0.75	0.945	0.894	0.845	0.799	0.755	0.714	0.675	0.638	0.603	0.570
0.76	0.944	0.891	0.841	0.794	0.749	0.707	0.667	0.630	0.595	0.561
0.77	0.942	0.888	0.837	0.789	0.743	0.701	0.660	0.622	0.586	0.553
0.78	0.941	0.885	0.833	0.784	0.738	0.694	0.653	0.615	0.578	0.544
0.79	0.939	0.883	0.829	0.779	0.732	0.688	0.646	0.607	0.570	0.536
0.80	0.938	0.880	0.825	0.774	0.726	0.681	0.639	0.599	0.562	0.527
0.81	0.936	0.877	0.821	0.769	0.720	0.675	0.632	0.592	0.554	0.519
0.82	0.935	0.874	0.817	0.764	0.714	0.668	0.625	0.584	0.546	0.510
0.83	0.933	0.871	0.813	0.759	0.709	0.661	0.617	0.576	0.538	0.502
0.84	0.932	0.868	0.809	0.754	0.703	0.655	0.610	0.569	0.530	0.494
0.85	0.930	0.865	0.805	0.749	0.697	0.648	0.603	0.561	0.522	0.486
0.86	0.929	0.863	0.801	0.744	0.691	0.642	0.596	0.553	0.514	0.477
0.87	0.927	0.860	0.797	0.739	0.685	0.635	0.589	0.546	0.506	0.469
0.88	0.925	0.857	0.793	0.734	0.679	0.628	0.582	0.538	0.498	0.461
0.89	0.924	0.853	0.788	0.728	0.673	0.622	0.574	0.531	0.490	0.453
0.90	0.922	0.850	0.784	0.723	0.667	0.615	0.567	0.523	0.482	0.445
0.91	0.921	0.847	0.780	0.718	0.661	0.608	0.560	0.516	0.475	0.437
0.92	0.919	0.844	0.776	0.713	0.655	0.602	0.553	0.508	0.467	0.429
0.93	0.917	0.841	0.771	0.708	0.649	0.595	0.546	0.501	0.459	0.421
0.94	0.915	0.838	0.767	0.702	0.643	0.589	0.539	0.493	0.451	0.413
0.95	0.914	0.835	0.763	0.697	0.637	0.582	0.532	0.486	0.444	0.406
0.96	0.912	0.832	0.758	0.692	0.631	0.575	0.525	0.478	0.436	0.398
0.97	0.910	0.828	0.754	0.686	0.625	0.569	0.518	0.471	0.429	0.390
0.98	0.908	0.825	0.750	0.681	0.619	0.562	0.511	0.464	0.421	0.383
0.99	0.907	0.822	0.745	0.676	0.613	0.555	0.504	0.457	0.414	0.375
1.00	0.905	0.819	0.741	0.670	0.607	0.549	0.497	0.449	0.407	0.368

TABLE 5.2.2A (continued)

$$\exp(-B \sin^2 \theta / \lambda^2)$$

$\frac{\sin \theta}{\lambda}$	$B=0.1$	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
1.01	0.903	0.815	0.736	0.665	0.600	0.542	0.490	0.442	0.399	0.361
1.02	0.901	0.812	0.732	0.660	0.594	0.536	0.483	0.435	0.392	0.353
1.03	0.899	0.809	0.727	0.654	0.588	0.529	0.476	0.428	0.385	0.346
1.04	0.897	0.805	0.723	0.649	0.582	0.523	0.469	0.421	0.378	0.339
1.05	0.896	0.802	0.718	0.643	0.576	0.516	0.462	0.414	0.371	0.332
1.06	0.894	0.799	0.714	0.638	0.570	0.510	0.455	0.407	0.364	0.325
1.07	0.892	0.795	0.709	0.633	0.564	0.503	0.449	0.400	0.357	0.318
1.08	0.890	0.792	0.705	0.627	0.558	0.497	0.442	0.393	0.350	0.311
1.09	0.888	0.789	0.700	0.622	0.552	0.490	0.435	0.387	0.343	0.305
1.10	0.886	0.785	0.696	0.616	0.546	0.484	0.429	0.380	0.337	0.298
1.11	0.884	0.782	0.691	0.611	0.540	0.477	0.422	0.373	0.330	0.292
1.12	0.882	0.778	0.686	0.605	0.534	0.471	0.416	0.367	0.323	0.285
1.13	0.880	0.775	0.682	0.600	0.528	0.465	0.409	0.360	0.317	0.279
1.14	0.878	0.771	0.677	0.595	0.522	0.459	0.403	0.354	0.310	0.273
1.15	0.876	0.768	0.673	0.589	0.516	0.452	0.396	0.347	0.304	0.266
1.16	0.874	0.764	0.668	0.584	0.510	0.446	0.390	0.341	0.298	0.260
1.17	0.872	0.760	0.663	0.578	0.504	0.440	0.384	0.334	0.292	0.254
1.18	0.870	0.757	0.659	0.573	0.498	0.434	0.377	0.328	0.286	0.248
1.19	0.868	0.753	0.654	0.568	0.493	0.428	0.371	0.322	0.280	0.243
1.20	0.866	0.750	0.649	0.562	0.487	0.421	0.365	0.316	0.274	0.237
1.21	0.864	0.746	0.645	0.557	0.481	0.415	0.359	0.310	0.268	0.231
1.22	0.862	0.743	0.640	0.551	0.475	0.409	0.353	0.304	0.262	0.226
1.23	0.860	0.739	0.635	0.546	0.469	0.403	0.347	0.298	0.256	0.220
1.24	0.857	0.735	0.630	0.541	0.464	0.398	0.341	0.292	0.251	0.215
1.25	0.855	0.732	0.626	0.535	0.458	0.392	0.335	0.287	0.245	0.210
1.26	0.853	0.728	0.621	0.530	0.452	0.386	0.329	0.281	0.240	0.204
1.27	0.851	0.724	0.616	0.525	0.446	0.380	0.323	0.275	0.234	0.199
1.28	0.849	0.721	0.612	0.519	0.441	0.374	0.318	0.270	0.229	0.194
1.29	0.847	0.717	0.607	0.514	0.435	0.368	0.312	0.264	0.224	0.189
1.30	0.845	0.713	0.602	0.509	0.430	0.363	0.306	0.259	0.218	0.185
1.31	0.842	0.709	0.598	0.503	0.424	0.357	0.301	0.253	0.213	0.180
1.32	0.840	0.706	0.593	0.498	0.418	0.352	0.295	0.248	0.208	0.175
1.33	0.838	0.702	0.588	0.493	0.413	0.346	0.290	0.243	0.204	0.171
1.34	0.836	0.698	0.584	0.488	0.407	0.340	0.285	0.238	0.199	0.166
1.35	0.833	0.695	0.579	0.482	0.402	0.335	0.279	0.233	0.194	0.162
1.36	0.831	0.691	0.574	0.477	0.397	0.330	0.274	0.228	0.189	0.157
1.37	0.829	0.687	0.569	0.472	0.391	0.324	0.269	0.223	0.185	0.153
1.38	0.827	0.683	0.565	0.467	0.386	0.319	0.264	0.218	0.180	0.149
1.39	0.824	0.679	0.560	0.462	0.381	0.314	0.259	0.213	0.176	0.145
1.40	0.822	0.676	0.555	0.457	0.375	0.309	0.254	0.208	0.171	0.141
1.41	0.820	0.672	0.551	0.451	0.370	0.303	0.249	0.204	0.167	0.137
1.42	0.817	0.668	0.546	0.446	0.365	0.298	0.244	0.199	0.163	0.133
1.43	0.815	0.664	0.541	0.441	0.360	0.293	0.239	0.195	0.159	0.129
1.44	0.813	0.661	0.537	0.436	0.355	0.288	0.234	0.190	0.155	0.126
1.45	0.810	0.657	0.532	0.431	0.350	0.283	0.230	0.186	0.151	0.122
1.46	0.808	0.653	0.528	0.426	0.344	0.278	0.225	0.182	0.147	0.119
1.47	0.806	0.649	0.523	0.421	0.339	0.273	0.220	0.178	0.143	0.115
1.48	0.803	0.645	0.518	0.416	0.334	0.269	0.216	0.173	0.139	0.112
1.49	0.801	0.641	0.514	0.411	0.330	0.264	0.211	0.169	0.136	0.109
1.50	0.799	0.638	0.509	0.407	0.325	0.259	0.207	0.165	0.132	0.105

TABLE 5.2.2A (continued)

 $\exp(-B \sin^2 \theta / \lambda^2)$

$\frac{\sin \theta}{\lambda}$	$B=1.1$	1.2	1.3	1.4	1.5	1.6	1.7	1.8	1.9	2.0
0.01	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.02	1.000	1.000	0.999	0.999	0.999	0.999	0.999	0.999	0.999	0.999
0.03	0.999	0.999	0.999	0.999	0.999	0.999	0.998	0.998	0.998	0.998
0.04	0.998	0.998	0.998	0.998	0.998	0.997	0.997	0.997	0.997	0.997
0.05	0.997	0.997	0.997	0.997	0.996	0.996	0.996	0.996	0.995	0.995
0.06	0.996	0.996	0.995	0.995	0.995	0.994	0.994	0.994	0.993	0.993
0.07	0.995	0.994	0.994	0.993	0.993	0.992	0.992	0.991	0.991	0.990
0.08	0.993	0.992	0.992	0.991	0.990	0.990	0.989	0.989	0.988	0.987
0.09	0.991	0.990	0.990	0.989	0.988	0.987	0.986	0.986	0.985	0.984
0.10	0.989	0.988	0.987	0.986	0.985	0.984	0.983	0.982	0.981	0.980
0.11	0.987	0.986	0.984	0.983	0.982	0.981	0.980	0.978	0.977	0.976
0.12	0.984	0.983	0.981	0.980	0.979	0.977	0.976	0.974	0.973	0.972
0.13	0.982	0.980	0.978	0.977	0.975	0.973	0.972	0.970	0.968	0.967
0.14	0.979	0.977	0.975	0.973	0.971	0.969	0.967	0.965	0.963	0.962
0.15	0.976	0.973	0.971	0.969	0.967	0.965	0.962	0.960	0.958	0.956
0.16	0.972	0.970	0.967	0.965	0.962	0.960	0.957	0.955	0.953	0.950
0.17	0.969	0.966	0.963	0.960	0.958	0.955	0.952	0.949	0.947	0.944
0.18	0.965	0.962	0.959	0.956	0.953	0.949	0.946	0.943	0.940	0.937
0.19	0.961	0.958	0.954	0.951	0.947	0.944	0.940	0.937	0.934	0.930
0.20	0.957	0.953	0.949	0.946	0.942	0.938	0.934	0.931	0.927	0.923
0.21	0.953	0.948	0.944	0.940	0.936	0.932	0.928	0.924	0.920	0.916
0.22	0.948	0.944	0.939	0.934	0.930	0.925	0.921	0.917	0.912	0.908
0.23	0.943	0.938	0.934	0.929	0.924	0.919	0.914	0.909	0.904	0.900
0.24	0.939	0.933	0.928	0.923	0.917	0.912	0.907	0.902	0.896	0.891
0.25	0.934	0.928	0.922	0.916	0.911	0.905	0.899	0.894	0.888	0.882
0.26	0.928	0.922	0.916	0.910	0.904	0.897	0.891	0.885	0.879	0.874
0.27	0.923	0.916	0.910	0.903	0.896	0.890	0.883	0.877	0.871	0.864
0.28	0.917	0.910	0.903	0.896	0.889	0.882	0.875	0.868	0.862	0.855
0.29	0.912	0.904	0.896	0.889	0.881	0.874	0.867	0.860	0.852	0.845
0.30	0.906	0.898	0.890	0.882	0.874	0.866	0.858	0.850	0.843	0.835
0.31	0.900	0.891	0.883	0.874	0.866	0.857	0.849	0.841	0.833	0.825
0.32	0.893	0.884	0.875	0.866	0.858	0.849	0.840	0.832	0.823	0.815
0.33	0.887	0.877	0.868	0.859	0.849	0.840	0.831	0.822	0.813	0.804
0.34	0.881	0.870	0.860	0.851	0.841	0.831	0.822	0.812	0.803	0.794
0.35	0.874	0.863	0.853	0.842	0.832	0.822	0.812	0.802	0.792	0.783
0.36	0.867	0.856	0.845	0.834	0.823	0.813	0.802	0.792	0.782	0.772
0.37	0.860	0.849	0.837	0.826	0.814	0.803	0.792	0.782	0.771	0.760
0.38	0.853	0.841	0.829	0.817	0.805	0.794	0.782	0.771	0.760	0.749
0.39	0.846	0.833	0.821	0.808	0.796	0.784	0.772	0.760	0.749	0.738
0.40	0.839	0.825	0.812	0.799	0.787	0.774	0.762	0.750	0.738	0.726
0.41	0.831	0.817	0.804	0.790	0.777	0.764	0.751	0.739	0.727	0.714
0.42	0.824	0.809	0.795	0.781	0.768	0.754	0.741	0.728	0.715	0.703
0.43	0.816	0.801	0.786	0.772	0.758	0.744	0.730	0.717	0.704	0.691
0.44	0.808	0.793	0.777	0.763	0.748	0.734	0.720	0.706	0.692	0.679
0.45	0.800	0.784	0.769	0.753	0.738	0.723	0.709	0.695	0.681	0.667
0.46	0.792	0.776	0.760	0.744	0.728	0.713	0.698	0.683	0.669	0.655
0.47	0.784	0.767	0.750	0.734	0.718	0.702	0.687	0.672	0.657	0.643
0.48	0.776	0.758	0.741	0.724	0.708	0.692	0.676	0.661	0.645	0.631
0.49	0.768	0.750	0.732	0.715	0.698	0.681	0.665	0.649	0.634	0.619
0.50	0.760	0.741	0.723	0.705	0.687	0.670	0.654	0.638	0.622	0.607

TABLE 5.2.2A (continued)

 $\exp(-B \sin^2 \theta / \lambda^2)$

$\frac{\sin \theta}{\lambda}$	$B=1.1$	1.2	1.3	1.4	1.5	1.6	1.7	1.8	1.9	2.0
0.51	0.751	0.732	0.713	0.695	0.677	0.660	0.643	0.626	0.610	0.594
0.52	0.743	0.723	0.704	0.685	0.667	0.649	0.631	0.615	0.598	0.582
0.53	0.734	0.714	0.694	0.675	0.656	0.638	0.620	0.603	0.586	0.570
0.54	0.726	0.705	0.684	0.665	0.646	0.627	0.609	0.592	0.575	0.558
0.55	0.717	0.696	0.675	0.655	0.635	0.616	0.598	0.580	0.563	0.546
0.56	0.708	0.686	0.665	0.645	0.625	0.605	0.587	0.569	0.551	0.534
0.57	0.699	0.677	0.655	0.635	0.614	0.595	0.576	0.557	0.539	0.522
0.58	0.691	0.668	0.646	0.624	0.604	0.584	0.564	0.546	0.528	0.510
0.59	0.682	0.659	0.636	0.614	0.593	0.573	0.553	0.534	0.516	0.498
0.60	0.673	0.649	0.626	0.604	0.583	0.562	0.542	0.523	0.505	0.487
0.61	0.664	0.640	0.616	0.594	0.572	0.551	0.531	0.512	0.493	0.475
0.62	0.655	0.630	0.607	0.584	0.562	0.541	0.520	0.501	0.482	0.464
0.63	0.646	0.621	0.597	0.574	0.551	0.530	0.509	0.489	0.470	0.452
0.64	0.637	0.612	0.587	0.564	0.541	0.519	0.498	0.478	0.459	0.441
0.65	0.628	0.602	0.577	0.553	0.531	0.509	0.488	0.467	0.448	0.430
0.66	0.619	0.593	0.568	0.543	0.520	0.498	0.477	0.457	0.437	0.418
0.67	0.610	0.584	0.558	0.533	0.510	0.488	0.466	0.446	0.426	0.407
0.68	0.601	0.574	0.548	0.523	0.500	0.477	0.456	0.435	0.415	0.397
0.69	0.592	0.565	0.539	0.513	0.490	0.467	0.445	0.424	0.405	0.386
0.70	0.583	0.555	0.529	0.504	0.480	0.457	0.435	0.414	0.394	0.375
0.71	0.574	0.546	0.519	0.494	0.469	0.446	0.424	0.404	0.384	0.365
0.72	0.565	0.537	0.510	0.484	0.460	0.436	0.414	0.393	0.373	0.355
0.73	0.556	0.528	0.500	0.474	0.450	0.426	0.404	0.383	0.363	0.344
0.74	0.548	0.518	0.491	0.465	0.440	0.416	0.394	0.373	0.353	0.334
0.75	0.539	0.509	0.481	0.455	0.430	0.407	0.384	0.363	0.343	0.325
0.76	0.530	0.500	0.472	0.445	0.420	0.397	0.375	0.354	0.334	0.315
0.77	0.521	0.491	0.463	0.436	0.411	0.387	0.365	0.344	0.324	0.306
0.78	0.512	0.482	0.453	0.427	0.401	0.378	0.355	0.334	0.315	0.296
0.79	0.503	0.473	0.444	0.417	0.392	0.368	0.346	0.325	0.306	0.287
0.80	0.495	0.464	0.435	0.408	0.383	0.359	0.337	0.316	0.296	0.278
0.81	0.486	0.455	0.426	0.399	0.374	0.350	0.328	0.307	0.287	0.269
0.82	0.477	0.446	0.417	0.390	0.365	0.341	0.319	0.298	0.279	0.261
0.83	0.469	0.437	0.408	0.381	0.356	0.332	0.310	0.289	0.270	0.252
0.84	0.460	0.429	0.400	0.372	0.347	0.323	0.301	0.281	0.262	0.244
0.85	0.452	0.420	0.391	0.364	0.338	0.315	0.293	0.272	0.253	0.236
0.86	0.443	0.412	0.382	0.355	0.330	0.306	0.284	0.264	0.245	0.228
0.87	0.435	0.403	0.374	0.347	0.321	0.298	0.276	0.256	0.237	0.220
0.88	0.427	0.395	0.365	0.338	0.313	0.290	0.268	0.248	0.230	0.213
0.89	0.418	0.387	0.357	0.330	0.305	0.282	0.260	0.240	0.222	0.205
0.90	0.410	0.378	0.349	0.322	0.297	0.274	0.252	0.233	0.215	0.198
0.91	0.402	0.370	0.341	0.314	0.289	0.266	0.245	0.225	0.207	0.191
0.92	0.394	0.362	0.333	0.306	0.281	0.258	0.237	0.218	0.200	0.184
0.93	0.386	0.354	0.325	0.298	0.273	0.251	0.230	0.211	0.193	0.177
0.94	0.378	0.346	0.317	0.290	0.266	0.243	0.223	0.204	0.187	0.171
0.95	0.371	0.339	0.309	0.283	0.258	0.236	0.216	0.197	0.180	0.164
0.96	0.363	0.331	0.302	0.275	0.251	0.229	0.209	0.190	0.174	0.158
0.97	0.355	0.323	0.294	0.268	0.244	0.222	0.202	0.184	0.167	0.152
0.98	0.348	0.316	0.287	0.261	0.237	0.215	0.195	0.178	0.161	0.146
0.99	0.340	0.308	0.280	0.254	0.230	0.208	0.189	0.171	0.155	0.141
1.00	0.333	0.301	0.273	0.247	0.223	0.202	0.183	0.165	0.150	0.135

TABLE 5.2.2A (continued)

 $\exp(-B \sin^2 \theta / \lambda^2)$

$\frac{\sin \theta}{\lambda}$	$B=1.1$	1.2	1.3	1.4	1.5	1.6	1.7	1.8	1.9	2.0
1.01	0.326	0.294	0.266	0.240	0.217	0.196	0.177	0.159	0.144	0.130
1.02	0.318	0.287	0.259	0.233	0.210	0.189	0.171	0.154	0.139	0.125
1.03	0.311	0.280	0.252	0.226	0.204	0.183	0.165	0.148	0.133	0.120
1.04	0.304	0.273	0.245	0.220	0.197	0.177	0.159	0.143	0.128	0.115
1.05	0.297	0.266	0.239	0.214	0.191	0.171	0.153	0.137	0.123	0.110
1.06	0.291	0.260	0.232	0.207	0.185	0.166	0.148	0.132	0.118	0.106
1.07	0.284	0.253	0.226	0.201	0.180	0.160	0.143	0.127	0.114	0.101
1.08	0.277	0.247	0.220	0.195	0.174	0.155	0.138	0.123	0.109	0.097
1.09	0.271	0.240	0.213	0.190	0.168	0.149	0.133	0.118	0.105	0.093
1.10	0.264	0.234	0.207	0.184	0.163	0.144	0.128	0.113	0.100	0.089
1.11	0.258	0.228	0.202	0.178	0.158	0.139	0.123	0.109	0.096	0.085
1.12	0.252	0.222	0.196	0.173	0.152	0.134	0.119	0.105	0.092	0.081
1.13	0.245	0.216	0.190	0.167	0.147	0.130	0.114	0.100	0.088	0.078
1.14	0.239	0.210	0.185	0.162	0.142	0.125	0.110	0.096	0.085	0.074
1.15	0.233	0.205	0.179	0.157	0.138	0.121	0.106	0.093	0.081	0.071
1.16	0.228	0.199	0.174	0.152	0.133	0.116	0.102	0.089	0.078	0.068
1.17	0.222	0.193	0.169	0.147	0.128	0.112	0.098	0.085	0.074	0.065
1.18	0.216	0.188	0.164	0.142	0.124	0.108	0.094	0.082	0.071	0.062
1.19	0.211	0.183	0.159	0.138	0.120	0.104	0.090	0.078	0.068	0.059
1.20	0.205	0.178	0.154	0.133	0.115	0.100	0.086	0.075	0.065	0.056
1.21	0.200	0.173	0.149	0.129	0.111	0.096	0.083	0.072	0.062	0.053
1.22	0.195	0.168	0.144	0.124	0.107	0.092	0.080	0.069	0.059	0.051
1.23	0.189	0.163	0.140	0.120	0.103	0.089	0.076	0.066	0.056	0.049
1.24	0.184	0.158	0.135	0.116	0.100	0.085	0.073	0.063	0.054	0.046
1.25	0.179	0.153	0.131	0.112	0.096	0.082	0.070	0.060	0.051	0.044
1.26	0.174	0.149	0.127	0.108	0.092	0.079	0.067	0.057	0.049	0.042
1.27	0.170	0.144	0.123	0.105	0.089	0.076	0.064	0.055	0.047	0.040
1.28	0.165	0.140	0.119	0.101	0.086	0.073	0.062	0.052	0.044	0.038
1.29	0.160	0.136	0.115	0.097	0.082	0.070	0.059	0.050	0.042	0.036
1.30	0.156	0.132	0.111	0.094	0.079	0.067	0.057	0.048	0.040	0.034
1.31	0.151	0.128	0.107	0.090	0.076	0.064	0.054	0.046	0.038	0.032
1.32	0.147	0.124	0.104	0.087	0.073	0.062	0.052	0.043	0.036	0.031
1.33	0.143	0.120	0.100	0.084	0.070	0.059	0.049	0.041	0.035	0.029
1.34	0.139	0.116	0.097	0.081	0.068	0.057	0.047	0.039	0.033	0.028
1.35	0.135	0.112	0.094	0.078	0.065	0.054	0.045	0.038	0.031	0.026
1.36	0.131	0.109	0.090	0.075	0.062	0.052	0.043	0.036	0.030	0.025
1.37	0.127	0.105	0.087	0.072	0.060	0.050	0.041	0.034	0.028	0.023
1.38	0.123	0.102	0.084	0.070	0.057	0.047	0.039	0.032	0.027	0.022
1.39	0.119	0.098	0.081	0.067	0.055	0.045	0.037	0.031	0.025	0.021
1.40	0.116	0.095	0.078	0.064	0.053	0.043	0.036	0.029	0.024	0.020
1.41	0.112	0.092	0.075	0.062	0.051	0.042	0.034	0.028	0.023	0.019
1.42	0.109	0.089	0.073	0.059	0.049	0.040	0.032	0.027	0.022	0.018
1.43	0.105	0.086	0.070	0.057	0.047	0.038	0.031	0.025	0.021	0.017
1.44	0.102	0.083	0.067	0.055	0.045	0.036	0.029	0.024	0.019	0.016
1.45	0.099	0.080	0.065	0.053	0.043	0.035	0.028	0.023	0.018	0.015
1.46	0.096	0.077	0.063	0.051	0.041	0.033	0.027	0.022	0.017	0.014
1.47	0.093	0.075	0.060	0.049	0.039	0.032	0.025	0.020	0.016	0.013
1.48	0.090	0.072	0.058	0.047	0.037	0.030	0.024	0.019	0.016	0.013
1.49	0.087	0.070	0.056	0.045	0.036	0.029	0.023	0.018	0.015	0.012
1.50	0.084	0.067	0.054	0.043	0.034	0.027	0.022	0.017	0.014	0.011

TABLE 5.2.2A (continued)

$$\exp(-B \sin^2 \theta / \lambda^2)$$

$\frac{\sin \theta}{\lambda}$	$B=2.1$	2.2	2.3	2.4	2.5	2.6	2.7	2.8	2.9	3.0
0.01	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.02	0.999	0.999	0.999	0.999	0.999	0.999	0.999	0.999	0.999	0.999
0.03	0.998	0.998	0.998	0.998	0.998	0.998	0.998	0.997	0.997	0.997
0.04	0.997	0.996	0.996	0.996	0.996	0.996	0.996	0.996	0.995	0.995
0.05	0.995	0.995	0.994	0.994	0.994	0.994	0.993	0.993	0.993	0.993
0.06	0.992	0.992	0.992	0.991	0.991	0.991	0.990	0.990	0.990	0.989
0.07	0.990	0.989	0.989	0.988	0.988	0.987	0.987	0.986	0.986	0.985
0.08	0.987	0.986	0.985	0.985	0.984	0.983	0.983	0.982	0.982	0.981
0.09	0.983	0.982	0.982	0.981	0.980	0.979	0.978	0.978	0.977	0.976
0.10	0.979	0.978	0.977	0.976	0.975	0.974	0.973	0.972	0.971	0.970
0.11	0.975	0.974	0.973	0.971	0.970	0.969	0.968	0.967	0.966	0.964
0.12	0.970	0.969	0.967	0.966	0.965	0.963	0.962	0.960	0.959	0.958
0.13	0.965	0.964	0.962	0.960	0.959	0.957	0.955	0.954	0.952	0.951
0.14	0.960	0.958	0.956	0.954	0.952	0.950	0.948	0.947	0.945	0.943
0.15	0.954	0.952	0.950	0.947	0.945	0.943	0.941	0.939	0.937	0.935
0.16	0.948	0.945	0.943	0.940	0.938	0.936	0.933	0.931	0.928	0.926
0.17	0.941	0.938	0.936	0.933	0.930	0.928	0.925	0.922	0.920	0.917
0.18	0.934	0.931	0.928	0.925	0.922	0.919	0.916	0.913	0.910	0.907
0.19	0.927	0.924	0.920	0.917	0.914	0.910	0.907	0.904	0.901	0.897
0.20	0.919	0.916	0.912	0.908	0.905	0.901	0.898	0.894	0.890	0.887
0.21	0.912	0.908	0.904	0.900	0.896	0.892	0.888	0.884	0.880	0.876
0.22	0.903	0.899	0.895	0.890	0.886	0.882	0.877	0.873	0.869	0.865
0.23	0.895	0.890	0.885	0.881	0.876	0.871	0.867	0.862	0.858	0.853
0.24	0.886	0.881	0.876	0.871	0.866	0.861	0.856	0.851	0.846	0.841
0.25	0.877	0.872	0.866	0.861	0.855	0.850	0.845	0.839	0.834	0.829
0.26	0.868	0.862	0.856	0.850	0.845	0.839	0.833	0.828	0.822	0.816
0.27	0.858	0.852	0.846	0.839	0.833	0.827	0.821	0.815	0.809	0.804
0.28	0.848	0.842	0.835	0.828	0.822	0.816	0.809	0.803	0.797	0.790
0.29	0.838	0.831	0.824	0.817	0.810	0.804	0.797	0.790	0.784	0.777
0.30	0.828	0.820	0.813	0.806	0.799	0.791	0.784	0.777	0.770	0.763
0.31	0.817	0.809	0.802	0.794	0.786	0.779	0.771	0.764	0.757	0.750
0.32	0.807	0.798	0.790	0.782	0.774	0.766	0.758	0.751	0.743	0.736
0.33	0.796	0.787	0.778	0.770	0.762	0.753	0.745	0.737	0.729	0.721
0.34	0.784	0.775	0.767	0.758	0.749	0.740	0.732	0.723	0.715	0.707
0.35	0.773	0.764	0.754	0.745	0.736	0.727	0.718	0.710	0.701	0.692
0.36	0.762	0.752	0.742	0.733	0.723	0.714	0.705	0.696	0.687	0.678
0.37	0.750	0.740	0.730	0.720	0.710	0.701	0.691	0.682	0.672	0.663
0.38	0.738	0.728	0.717	0.707	0.697	0.687	0.677	0.667	0.658	0.648
0.39	0.727	0.716	0.705	0.694	0.684	0.673	0.663	0.653	0.643	0.634
0.40	0.715	0.703	0.692	0.681	0.670	0.660	0.649	0.639	0.629	0.619
0.41	0.703	0.691	0.679	0.668	0.657	0.646	0.635	0.625	0.614	0.604
0.42	0.690	0.678	0.666	0.655	0.643	0.632	0.621	0.610	0.600	0.589
0.43	0.678	0.666	0.654	0.642	0.630	0.618	0.607	0.596	0.585	0.574
0.44	0.666	0.653	0.641	0.628	0.616	0.604	0.593	0.582	0.570	0.559
0.45	0.654	0.641	0.628	0.615	0.603	0.591	0.579	0.567	0.556	0.545
0.46	0.641	0.628	0.615	0.602	0.589	0.577	0.565	0.553	0.541	0.530
0.47	0.629	0.615	0.602	0.589	0.576	0.563	0.551	0.539	0.527	0.515
0.48	0.616	0.602	0.589	0.575	0.562	0.549	0.537	0.525	0.513	0.501
0.49	0.604	0.590	0.576	0.562	0.549	0.536	0.523	0.511	0.498	0.487
0.50	0.592	0.577	0.563	0.549	0.535	0.522	0.509	0.497	0.484	0.472

TABLE 5.2.2A (continued)

 $\exp(-B \sin^2 \theta/\lambda^2)$

$\frac{\sin \theta}{\lambda}$	$B=2.1$	2.2	2.3	2.4	2.5	2.6	2.7	2.8	2.9	3.0
0.51	0.579	0.564	0.550	0.536	0.522	0.509	0.495	0.483	0.470	0.458
0.52	0.567	0.552	0.537	0.523	0.509	0.495	0.482	0.469	0.457	0.444
0.53	0.554	0.539	0.524	0.510	0.495	0.482	0.468	0.455	0.443	0.431
0.54	0.542	0.526	0.511	0.497	0.482	0.469	0.455	0.442	0.429	0.417
0.55	0.530	0.514	0.499	0.484	0.469	0.455	0.442	0.429	0.416	0.404
0.56	0.518	0.502	0.486	0.471	0.457	0.442	0.429	0.416	0.403	0.390
0.57	0.505	0.489	0.474	0.459	0.444	0.430	0.416	0.403	0.390	0.377
0.58	0.493	0.477	0.461	0.446	0.431	0.417	0.403	0.390	0.377	0.365
0.59	0.481	0.465	0.449	0.434	0.419	0.405	0.391	0.377	0.364	0.352
0.60	0.470	0.453	0.437	0.421	0.407	0.392	0.378	0.365	0.352	0.340
0.61	0.458	0.441	0.425	0.409	0.394	0.380	0.366	0.353	0.340	0.327
0.62	0.446	0.429	0.413	0.398	0.383	0.368	0.354	0.341	0.328	0.316
0.63	0.435	0.418	0.401	0.386	0.371	0.356	0.342	0.329	0.316	0.304
0.64	0.423	0.406	0.390	0.374	0.359	0.345	0.331	0.318	0.305	0.293
0.65	0.412	0.395	0.378	0.363	0.348	0.333	0.320	0.306	0.294	0.282
0.66	0.401	0.384	0.367	0.352	0.337	0.322	0.308	0.295	0.283	0.271
0.67	0.390	0.372	0.356	0.340	0.326	0.311	0.298	0.285	0.272	0.260
0.68	0.379	0.362	0.345	0.330	0.315	0.301	0.287	0.274	0.262	0.250
0.69	0.368	0.351	0.335	0.319	0.304	0.290	0.277	0.264	0.251	0.240
0.70	0.357	0.340	0.324	0.309	0.294	0.280	0.266	0.254	0.241	0.230
0.71	0.347	0.330	0.314	0.298	0.284	0.270	0.256	0.244	0.232	0.220
0.72	0.337	0.320	0.304	0.288	0.274	0.260	0.247	0.234	0.222	0.211
0.73	0.327	0.310	0.294	0.278	0.264	0.250	0.237	0.225	0.213	0.202
0.74	0.317	0.300	0.284	0.269	0.254	0.241	0.228	0.216	0.204	0.193
0.75	0.307	0.290	0.274	0.259	0.245	0.232	0.219	0.207	0.196	0.185
0.76	0.297	0.281	0.265	0.250	0.236	0.223	0.210	0.198	0.187	0.177
0.77	0.288	0.271	0.256	0.241	0.227	0.214	0.202	0.190	0.179	0.169
0.78	0.279	0.262	0.247	0.232	0.218	0.206	0.193	0.182	0.171	0.161
0.79	0.270	0.253	0.238	0.224	0.210	0.197	0.185	0.174	0.164	0.154
0.80	0.261	0.245	0.229	0.215	0.202	0.189	0.178	0.167	0.156	0.147
0.81	0.252	0.236	0.221	0.207	0.194	0.182	0.170	0.159	0.149	0.140
0.82	0.244	0.228	0.213	0.199	0.186	0.174	0.163	0.152	0.142	0.133
0.83	0.235	0.220	0.205	0.191	0.179	0.167	0.156	0.145	0.136	0.127
0.84	0.227	0.212	0.197	0.184	0.171	0.160	0.149	0.139	0.129	0.120
0.85	0.219	0.204	0.190	0.177	0.164	0.153	0.142	0.132	0.123	0.114
0.86	0.212	0.196	0.182	0.169	0.157	0.146	0.136	0.126	0.117	0.109
0.87	0.204	0.189	0.175	0.163	0.151	0.140	0.130	0.120	0.111	0.103
0.88	0.197	0.182	0.168	0.156	0.144	0.134	0.124	0.114	0.106	0.098
0.89	0.189	0.175	0.162	0.149	0.138	0.128	0.118	0.109	0.101	0.093
0.90	0.183	0.168	0.155	0.143	0.132	0.122	0.112	0.104	0.095	0.088
0.91	0.176	0.162	0.149	0.137	0.126	0.116	0.107	0.098	0.091	0.083
0.92	0.169	0.155	0.143	0.131	0.121	0.111	0.102	0.093	0.086	0.079
0.93	0.163	0.149	0.137	0.125	0.115	0.106	0.097	0.089	0.081	0.075
0.94	0.156	0.143	0.131	0.120	0.110	0.101	0.092	0.084	0.077	0.071
0.95	0.150	0.137	0.125	0.115	0.105	0.096	0.087	0.080	0.073	0.067
0.96	0.144	0.132	0.120	0.110	0.100	0.091	0.083	0.076	0.069	0.063
0.97	0.139	0.126	0.115	0.105	0.095	0.087	0.079	0.072	0.065	0.059
0.98	0.133	0.121	0.110	0.100	0.091	0.082	0.075	0.068	0.062	0.056
0.99	0.128	0.116	0.105	0.095	0.086	0.078	0.071	0.064	0.058	0.053
1.00	0.122	0.111	0.100	0.091	0.082	0.074	0.067	0.061	0.055	0.050

TABLE 5.2.2A (continued)

 $\exp(-B \sin^2 \theta / \lambda^2)$

$\frac{\sin \theta}{\lambda}$	$B=2.1$	2.2	2.3	2.4	2.5	2.6	2.7	2.8	2.9	3.0
1.01	0.117	0.106	0.096	0.086	0.078	0.070	0.064	0.057	0.052	0.047
1.02	0.112	0.101	0.091	0.082	0.074	0.067	0.060	0.054	0.049	0.044
1.03	0.108	0.097	0.087	0.078	0.070	0.063	0.057	0.051	0.046	0.041
1.04	0.103	0.093	0.083	0.075	0.067	0.060	0.054	0.048	0.043	0.039
1.05	0.099	0.088	0.079	0.071	0.064	0.057	0.051	0.046	0.041	0.037
1.06	0.094	0.084	0.075	0.067	0.060	0.054	0.048	0.043	0.038	0.034
1.07	0.090	0.081	0.072	0.064	0.057	0.051	0.045	0.041	0.036	0.032
1.08	0.086	0.077	0.068	0.061	0.054	0.048	0.043	0.038	0.034	0.030
1.09	0.082	0.073	0.065	0.058	0.051	0.046	0.040	0.036	0.032	0.028
1.10	0.079	0.070	0.062	0.055	0.049	0.043	0.038	0.034	0.030	0.027
1.11	0.075	0.066	0.059	0.052	0.046	0.041	0.036	0.032	0.028	0.025
1.12	0.072	0.063	0.056	0.049	0.043	0.038	0.034	0.030	0.026	0.023
1.13	0.068	0.060	0.053	0.047	0.041	0.036	0.032	0.028	0.025	0.022
1.14	0.065	0.057	0.050	0.044	0.039	0.034	0.030	0.026	0.023	0.020
1.15	0.062	0.055	0.048	0.042	0.037	0.032	0.028	0.025	0.022	0.019
1.16	0.059	0.052	0.045	0.040	0.035	0.030	0.026	0.023	0.020	0.018
1.17	0.056	0.049	0.043	0.037	0.033	0.028	0.025	0.022	0.019	0.016
1.18	0.054	0.047	0.041	0.035	0.031	0.027	0.023	0.020	0.018	0.015
1.19	0.051	0.044	0.039	0.033	0.029	0.025	0.022	0.019	0.016	0.014
1.20	0.049	0.042	0.037	0.032	0.027	0.024	0.020	0.018	0.015	0.013
1.21	0.046	0.040	0.035	0.030	0.026	0.022	0.019	0.017	0.014	0.012
1.22	0.044	0.038	0.033	0.028	0.024	0.021	0.018	0.015	0.013	0.012
1.23	0.042	0.036	0.031	0.026	0.023	0.020	0.017	0.014	0.012	0.011
1.24	0.040	0.034	0.029	0.025	0.021	0.018	0.016	0.013	0.012	0.010
1.25	0.038	0.032	0.027	0.024	0.020	0.017	0.015	0.013	0.011	0.009
1.26	0.036	0.030	0.026	0.022	0.019	0.016	0.014	0.012	0.010	0.009
1.27	0.034	0.029	0.024	0.021	0.018	0.015	0.013	0.011	0.009	0.008
1.28	0.032	0.027	0.023	0.020	0.017	0.014	0.012	0.010	0.009	0.007
1.29	0.030	0.026	0.022	0.018	0.016	0.013	0.011	0.009	0.008	0.007
1.30	0.029	0.024	0.021	0.017	0.015	0.012	0.010	0.009	0.007	0.006
1.31	0.027	0.023	0.019	0.016	0.014	0.012	0.010	0.008	0.007	0.006
1.32	0.026	0.022	0.018	0.015	0.013	0.011	0.009	0.008	0.006	0.005
1.33	0.024	0.020	0.017	0.014	0.012	0.010	0.008	0.007	0.006	0.005
1.34	0.023	0.019	0.016	0.013	0.011	0.009	0.008	0.007	0.005	0.005
1.35	0.022	0.018	0.015	0.013	0.011	0.009	0.007	0.006	0.005	0.004
1.36	0.021	0.017	0.014	0.012	0.010	0.008	0.007	0.006	0.005	0.004
1.37	0.019	0.016	0.013	0.011	0.009	0.008	0.006	0.005	0.004	0.004
1.38	0.018	0.015	0.013	0.010	0.009	0.007	0.006	0.005	0.004	0.003
1.39	0.017	0.014	0.012	0.010	0.008	0.007	0.005	0.004	0.004	0.003
1.40	0.016	0.013	0.011	0.009	0.007	0.006	0.005	0.004	0.003	0.003
1.41	0.015	0.013	0.010	0.008	0.007	0.006	0.005	0.004	0.003	0.003
1.42	0.014	0.012	0.010	0.008	0.006	0.005	0.004	0.004	0.003	0.002
1.43	0.014	0.011	0.009	0.007	0.006	0.005	0.004	0.003	0.003	0.002
1.44	0.013	0.010	0.008	0.007	0.006	0.005	0.004	0.003	0.002	0.002
1.45	0.012	0.010	0.008	0.006	0.005	0.004	0.003	0.003	0.002	0.002
1.46	0.011	0.009	0.007	0.006	0.005	0.004	0.003	0.003	0.002	0.002
1.47	0.011	0.009	0.007	0.006	0.005	0.004	0.003	0.002	0.002	0.002
1.48	0.010	0.008	0.006	0.005	0.004	0.003	0.003	0.002	0.002	0.001
1.49	0.009	0.008	0.006	0.005	0.004	0.003	0.002	0.002	0.002	0.001
1.50	0.009	0.007	0.006	0.005	0.004	0.003	0.002	0.002	0.001	0.001

TABLE 5.2.2A (continued)

 $\exp(-B \sin^2 \theta / \lambda^2)$

$\frac{\sin \theta}{\lambda}$	$B=3.1$	3.2	3.3	3.4	3.5	3.6	3.7	3.8	3.9	4.0
0.01	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.02	0.999	0.999	0.999	0.999	0.999	0.999	0.999	0.998	0.998	0.998
0.03	0.997	0.997	0.997	0.997	0.997	0.997	0.997	0.997	0.996	0.996
0.04	0.995	0.995	0.995	0.995	0.994	0.994	0.994	0.994	0.994	0.994
0.05	0.992	0.992	0.992	0.992	0.991	0.991	0.991	0.991	0.990	0.990
0.06	0.989	0.989	0.988	0.988	0.987	0.987	0.987	0.986	0.986	0.986
0.07	0.985	0.984	0.984	0.983	0.983	0.983	0.982	0.982	0.981	0.981
0.08	0.980	0.980	0.979	0.978	0.978	0.977	0.977	0.976	0.975	0.975
0.09	0.975	0.974	0.974	0.973	0.972	0.971	0.970	0.970	0.969	0.968
0.10	0.969	0.969	0.968	0.967	0.966	0.965	0.964	0.963	0.962	0.961
0.11	0.963	0.962	0.961	0.960	0.959	0.957	0.956	0.955	0.954	0.953
0.12	0.956	0.955	0.954	0.952	0.951	0.949	0.948	0.947	0.945	0.944
0.13	0.949	0.947	0.946	0.944	0.943	0.941	0.939	0.938	0.936	0.935
0.14	0.941	0.939	0.937	0.936	0.934	0.932	0.930	0.928	0.926	0.925
0.15	0.933	0.931	0.928	0.926	0.924	0.922	0.920	0.918	0.916	0.914
0.16	0.924	0.921	0.919	0.917	0.914	0.912	0.910	0.907	0.905	0.903
0.17	0.914	0.912	0.909	0.906	0.904	0.901	0.899	0.896	0.893	0.891
0.18	0.904	0.902	0.899	0.896	0.893	0.890	0.887	0.884	0.881	0.878
0.19	0.894	0.891	0.888	0.884	0.881	0.878	0.875	0.872	0.869	0.866
0.20	0.883	0.880	0.876	0.873	0.869	0.866	0.862	0.859	0.856	0.852
0.21	0.872	0.868	0.865	0.861	0.857	0.853	0.849	0.846	0.842	0.838
0.22	0.861	0.857	0.852	0.848	0.844	0.840	0.836	0.832	0.828	0.824
0.23	0.849	0.844	0.840	0.835	0.831	0.827	0.822	0.818	0.814	0.809
0.24	0.836	0.832	0.827	0.822	0.817	0.813	0.808	0.803	0.799	0.794
0.25	0.824	0.819	0.814	0.809	0.804	0.799	0.794	0.789	0.784	0.779
0.26	0.811	0.805	0.800	0.795	0.789	0.784	0.779	0.773	0.768	0.763
0.27	0.798	0.792	0.786	0.780	0.775	0.769	0.764	0.758	0.753	0.747
0.28	0.784	0.778	0.772	0.766	0.760	0.754	0.748	0.742	0.737	0.731
0.29	0.771	0.764	0.758	0.751	0.745	0.739	0.733	0.726	0.720	0.714
0.30	0.757	0.750	0.743	0.736	0.730	0.723	0.717	0.710	0.704	0.698
0.31	0.742	0.735	0.728	0.721	0.714	0.708	0.701	0.694	0.687	0.681
0.32	0.728	0.721	0.713	0.706	0.699	0.692	0.685	0.678	0.671	0.664
0.33	0.713	0.706	0.698	0.691	0.683	0.676	0.668	0.661	0.654	0.647
0.34	0.699	0.691	0.683	0.675	0.667	0.660	0.652	0.645	0.637	0.630
0.35	0.684	0.676	0.667	0.659	0.651	0.643	0.636	0.628	0.620	0.613
0.36	0.669	0.661	0.652	0.644	0.635	0.627	0.619	0.611	0.603	0.595
0.37	0.654	0.645	0.637	0.628	0.619	0.611	0.603	0.594	0.586	0.578
0.38	0.639	0.630	0.621	0.612	0.603	0.595	0.586	0.578	0.569	0.561
0.39	0.624	0.615	0.605	0.596	0.587	0.578	0.570	0.561	0.553	0.544
0.40	0.609	0.599	0.590	0.580	0.571	0.562	0.553	0.544	0.536	0.527
0.41	0.594	0.584	0.574	0.565	0.555	0.546	0.537	0.528	0.519	0.510
0.42	0.579	0.569	0.559	0.549	0.539	0.530	0.521	0.512	0.503	0.494
0.43	0.564	0.553	0.543	0.533	0.524	0.514	0.505	0.495	0.486	0.477
0.44	0.549	0.538	0.528	0.518	0.508	0.498	0.489	0.479	0.470	0.461
0.45	0.534	0.523	0.513	0.502	0.492	0.482	0.473	0.463	0.454	0.445
0.46	0.519	0.508	0.497	0.487	0.477	0.467	0.457	0.447	0.438	0.429
0.47	0.504	0.493	0.482	0.472	0.462	0.451	0.442	0.432	0.423	0.413
0.48	0.490	0.478	0.468	0.457	0.446	0.436	0.426	0.417	0.407	0.398
0.49	0.475	0.464	0.453	0.442	0.432	0.421	0.411	0.402	0.392	0.383
0.50	0.461	0.449	0.438	0.427	0.417	0.407	0.397	0.387	0.377	0.368

TABLE 5.2.2A (continued)

 $\exp(-B \sin^2 \theta/\lambda^2)$

$\frac{\sin \theta}{\lambda}$	$B=3.1$	3.2	3.3	3.4	3.5	3.6	3.7	3.8	3.9	4.0
0.51	0.447	0.435	0.424	0.413	0.402	0.392	0.382	0.372	0.363	0.353
0.52	0.432	0.421	0.410	0.399	0.388	0.378	0.368	0.358	0.348	0.339
0.53	0.419	0.407	0.396	0.385	0.374	0.364	0.354	0.344	0.334	0.325
0.54	0.405	0.393	0.382	0.371	0.360	0.350	0.340	0.330	0.321	0.311
0.55	0.392	0.380	0.369	0.358	0.347	0.337	0.327	0.317	0.307	0.298
0.56	0.378	0.367	0.355	0.344	0.334	0.323	0.313	0.304	0.294	0.285
0.57	0.365	0.354	0.342	0.331	0.321	0.310	0.301	0.291	0.282	0.273
0.58	0.352	0.341	0.330	0.319	0.308	0.298	0.288	0.279	0.269	0.260
0.59	0.340	0.328	0.317	0.306	0.296	0.286	0.276	0.266	0.257	0.248
0.60	0.328	0.316	0.305	0.294	0.284	0.274	0.264	0.255	0.246	0.237
0.61	0.316	0.304	0.293	0.282	0.272	0.262	0.252	0.243	0.234	0.226
0.62	0.304	0.292	0.281	0.271	0.260	0.251	0.241	0.232	0.223	0.215
0.63	0.292	0.281	0.270	0.259	0.249	0.240	0.230	0.221	0.213	0.204
0.64	0.281	0.270	0.259	0.248	0.238	0.229	0.220	0.211	0.202	0.194
0.65	0.270	0.259	0.248	0.238	0.228	0.218	0.209	0.201	0.192	0.185
0.66	0.259	0.248	0.238	0.227	0.218	0.208	0.200	0.191	0.183	0.175
0.67	0.249	0.238	0.227	0.217	0.208	0.199	0.190	0.182	0.174	0.166
0.68	0.238	0.228	0.217	0.208	0.198	0.189	0.181	0.173	0.165	0.157
0.69	0.229	0.218	0.208	0.198	0.189	0.180	0.172	0.164	0.156	0.149
0.70	0.219	0.208	0.198	0.189	0.180	0.171	0.163	0.155	0.148	0.141
0.71	0.210	0.199	0.189	0.180	0.171	0.163	0.155	0.147	0.140	0.133
0.72	0.200	0.190	0.181	0.172	0.163	0.155	0.147	0.139	0.132	0.126
0.73	0.192	0.182	0.172	0.163	0.155	0.147	0.139	0.132	0.125	0.119
0.74	0.183	0.173	0.164	0.155	0.147	0.139	0.132	0.125	0.118	0.112
0.75	0.175	0.165	0.156	0.148	0.140	0.132	0.125	0.118	0.112	0.105
0.76	0.167	0.158	0.149	0.140	0.132	0.125	0.118	0.111	0.105	0.099
0.77	0.159	0.150	0.141	0.133	0.126	0.118	0.112	0.105	0.099	0.093
0.78	0.152	0.143	0.134	0.126	0.119	0.112	0.105	0.099	0.093	0.088
0.79	0.144	0.136	0.128	0.120	0.113	0.106	0.099	0.093	0.088	0.082
0.80	0.138	0.129	0.121	0.113	0.106	0.100	0.094	0.088	0.082	0.077
0.81	0.131	0.123	0.115	0.107	0.101	0.094	0.088	0.083	0.077	0.072
0.82	0.124	0.116	0.109	0.102	0.095	0.089	0.083	0.078	0.073	0.068
0.83	0.118	0.110	0.103	0.096	0.090	0.084	0.078	0.073	0.068	0.064
0.84	0.112	0.105	0.097	0.091	0.085	0.079	0.073	0.068	0.064	0.059
0.85	0.106	0.099	0.092	0.086	0.080	0.074	0.069	0.064	0.060	0.056
0.86	0.101	0.094	0.087	0.081	0.075	0.070	0.065	0.060	0.056	0.052
0.87	0.096	0.089	0.082	0.076	0.071	0.066	0.061	0.056	0.052	0.048
0.88	0.091	0.084	0.078	0.072	0.067	0.062	0.057	0.053	0.049	0.045
0.89	0.086	0.079	0.073	0.068	0.063	0.058	0.053	0.049	0.046	0.042
0.90	0.081	0.075	0.069	0.064	0.059	0.054	0.050	0.046	0.042	0.039
0.95	0.061	0.056	0.051	0.046	0.042	0.039	0.035	0.032	0.030	0.027
1.00	0.045	0.041	0.037	0.033	0.030	0.027	0.025	0.022	0.020	0.018
1.05	0.033	0.029	0.026	0.024	0.021	0.019	0.017	0.015	0.014	0.012
1.10	0.023	0.021	0.018	0.016	0.014	0.013	0.011	0.010	0.009	0.008
1.15	0.017	0.015	0.013	0.011	0.010	0.009	0.007	0.007	0.006	0.005
1.20	0.012	0.010	0.009	0.007	0.006	0.006	0.005	0.004	0.004	0.003
1.25	0.008	0.007	0.006	0.005	0.004	0.004	0.003	0.003	0.002	0.002
1.30	0.005	0.004	0.004	0.003	0.003	0.002	0.002	0.002	0.001	0.001
1.40	0.002	0.002	0.002	0.001	0.001	0.001	0.001	0.001	0.000	0.000
1.50	0.001	0.001	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000

TABLE 5.2.2A (continued)
 $\exp(-B \sin^2 \theta / \lambda^2)$

$\frac{\sin \theta}{\lambda}$	$B=4.1$	4.2	4.3	4.4	4.5	4.6	4.7	4.8	4.9	5.0
0.01	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.02	0.998	0.998	0.998	0.998	0.998	0.998	0.998	0.998	0.998	0.998
0.03	0.996	0.996	0.996	0.996	0.996	0.996	0.996	0.996	0.996	0.996
0.04	0.993	0.993	0.993	0.993	0.993	0.993	0.993	0.992	0.992	0.992
0.05	0.990	0.990	0.989	0.989	0.989	0.989	0.988	0.988	0.988	0.988
0.06	0.985	0.985	0.985	0.984	0.984	0.984	0.983	0.983	0.983	0.982
0.07	0.980	0.980	0.979	0.979	0.978	0.978	0.977	0.977	0.976	0.976
0.08	0.974	0.973	0.973	0.972	0.972	0.971	0.970	0.970	0.969	0.969
0.09	0.967	0.967	0.966	0.965	0.964	0.963	0.963	0.962	0.961	0.960
0.10	0.960	0.959	0.958	0.957	0.956	0.955	0.954	0.953	0.952	0.951
0.11	0.952	0.950	0.949	0.948	0.947	0.946	0.945	0.944	0.942	0.941
0.12	0.943	0.941	0.940	0.939	0.937	0.936	0.935	0.933	0.932	0.931
0.13	0.933	0.931	0.930	0.928	0.927	0.925	0.924	0.922	0.921	0.919
0.14	0.923	0.921	0.919	0.917	0.916	0.914	0.912	0.910	0.908	0.907
0.15	0.912	0.910	0.908	0.906	0.904	0.902	0.900	0.898	0.896	0.894
0.16	0.900	0.898	0.896	0.893	0.891	0.889	0.887	0.884	0.882	0.880
0.17	0.888	0.886	0.883	0.881	0.878	0.876	0.873	0.870	0.868	0.865
0.18	0.876	0.873	0.870	0.867	0.864	0.862	0.859	0.856	0.853	0.850
0.19	0.862	0.859	0.856	0.853	0.850	0.847	0.844	0.841	0.838	0.835
0.20	0.849	0.845	0.842	0.839	0.835	0.832	0.829	0.825	0.822	0.819
0.21	0.835	0.831	0.827	0.824	0.820	0.816	0.813	0.809	0.806	0.802
0.22	0.820	0.816	0.812	0.808	0.804	0.800	0.797	0.793	0.789	0.785
0.23	0.805	0.801	0.797	0.792	0.788	0.784	0.780	0.776	0.772	0.768
0.24	0.790	0.785	0.781	0.776	0.772	0.767	0.763	0.758	0.754	0.750
0.25	0.774	0.769	0.764	0.760	0.755	0.750	0.745	0.741	0.736	0.732
0.26	0.758	0.753	0.748	0.743	0.738	0.733	0.728	0.723	0.718	0.713
0.27	0.742	0.736	0.731	0.726	0.720	0.715	0.710	0.705	0.700	0.695
0.28	0.725	0.719	0.714	0.708	0.703	0.697	0.692	0.686	0.681	0.676
0.29	0.708	0.702	0.697	0.691	0.685	0.679	0.673	0.668	0.662	0.657
0.30	0.691	0.685	0.679	0.673	0.667	0.661	0.655	0.649	0.643	0.638
0.31	0.674	0.668	0.662	0.655	0.649	0.643	0.637	0.630	0.624	0.618
0.32	0.657	0.650	0.644	0.637	0.631	0.624	0.618	0.612	0.605	0.599
0.33	0.640	0.633	0.626	0.619	0.613	0.606	0.599	0.593	0.586	0.580
0.34	0.623	0.615	0.608	0.601	0.594	0.588	0.581	0.574	0.568	0.561
0.35	0.605	0.598	0.591	0.583	0.576	0.569	0.562	0.555	0.549	0.542
0.36	0.588	0.580	0.573	0.565	0.558	0.551	0.544	0.537	0.530	0.523
0.37	0.570	0.563	0.555	0.548	0.540	0.533	0.525	0.518	0.511	0.504
0.38	0.553	0.545	0.537	0.530	0.522	0.515	0.507	0.500	0.493	0.486
0.39	0.536	0.528	0.520	0.512	0.504	0.497	0.489	0.482	0.475	0.467
0.40	0.519	0.511	0.503	0.495	0.487	0.479	0.471	0.464	0.457	0.449
0.41	0.502	0.494	0.485	0.477	0.469	0.462	0.454	0.446	0.439	0.431
0.42	0.485	0.477	0.468	0.460	0.452	0.444	0.436	0.429	0.421	0.414
0.43	0.469	0.460	0.452	0.443	0.435	0.427	0.419	0.412	0.404	0.397
0.44	0.452	0.443	0.435	0.427	0.418	0.410	0.403	0.395	0.387	0.380
0.45	0.436	0.427	0.419	0.410	0.402	0.394	0.386	0.378	0.371	0.363
0.46	0.420	0.411	0.403	0.394	0.386	0.378	0.370	0.362	0.355	0.347
0.47	0.404	0.395	0.387	0.378	0.370	0.362	0.354	0.346	0.339	0.331
0.48	0.389	0.380	0.371	0.363	0.355	0.347	0.339	0.331	0.323	0.316
0.49	0.374	0.365	0.356	0.348	0.339	0.331	0.324	0.316	0.308	0.301
0.50	0.359	0.350	0.341	0.333	0.325	0.317	0.309	0.301	0.294	0.287

TABLE 5.2.2A (continued)

 $\exp(-B \sin^2 \theta/\lambda^2)$

$\frac{\sin \theta}{\lambda}$	$B=4.1$	4.2	4.3	4.4	4.5	4.6	4.7	4.8	4.9	5.0
0.51	0.344	0.335	0.327	0.318	0.310	0.302	0.295	0.287	0.280	0.272
0.52	0.330	0.321	0.313	0.304	0.296	0.288	0.281	0.273	0.266	0.259
0.53	0.316	0.307	0.299	0.291	0.283	0.275	0.267	0.260	0.252	0.245
0.54	0.303	0.294	0.285	0.277	0.269	0.261	0.254	0.247	0.240	0.233
0.55	0.289	0.281	0.272	0.264	0.256	0.249	0.241	0.234	0.227	0.220
0.56	0.276	0.268	0.260	0.252	0.244	0.236	0.229	0.222	0.215	0.208
0.57	0.264	0.255	0.247	0.239	0.232	0.224	0.217	0.210	0.204	0.197
0.58	0.252	0.243	0.235	0.228	0.220	0.213	0.206	0.199	0.192	0.186
0.59	0.240	0.232	0.224	0.216	0.209	0.202	0.195	0.188	0.182	0.175
0.60	0.229	0.220	0.213	0.205	0.198	0.191	0.184	0.178	0.171	0.165
0.61	0.217	0.210	0.202	0.195	0.187	0.181	0.174	0.168	0.161	0.156
0.62	0.207	0.199	0.191	0.184	0.177	0.171	0.164	0.158	0.152	0.146
0.63	0.196	0.189	0.181	0.174	0.168	0.161	0.155	0.149	0.143	0.137
0.64	0.186	0.179	0.172	0.165	0.158	0.152	0.146	0.140	0.134	0.129
0.65	0.177	0.170	0.163	0.156	0.149	0.143	0.137	0.132	0.126	0.121
0.66	0.168	0.160	0.154	0.147	0.141	0.135	0.129	0.124	0.118	0.113
0.67	0.159	0.152	0.145	0.139	0.133	0.127	0.121	0.116	0.111	0.106
0.68	0.150	0.143	0.137	0.131	0.125	0.119	0.114	0.109	0.104	0.099
0.69	0.142	0.135	0.129	0.123	0.117	0.112	0.107	0.102	0.097	0.093
0.70	0.134	0.128	0.122	0.116	0.110	0.105	0.100	0.095	0.091	0.086
0.71	0.127	0.120	0.114	0.109	0.103	0.098	0.094	0.089	0.085	0.080
0.72	0.119	0.113	0.108	0.102	0.097	0.092	0.087	0.083	0.079	0.075
0.73	0.112	0.107	0.101	0.096	0.091	0.086	0.082	0.077	0.073	0.070
0.74	0.106	0.100	0.095	0.090	0.085	0.081	0.076	0.072	0.068	0.065
0.75	0.100	0.094	0.089	0.084	0.080	0.075	0.071	0.067	0.064	0.060
0.76	0.094	0.088	0.083	0.079	0.074	0.070	0.066	0.063	0.059	0.056
0.77	0.088	0.083	0.078	0.074	0.069	0.065	0.062	0.058	0.055	0.052
0.78	0.083	0.078	0.073	0.069	0.065	0.061	0.057	0.054	0.051	0.048
0.79	0.077	0.073	0.068	0.064	0.060	0.057	0.053	0.050	0.047	0.044
0.80	0.073	0.068	0.064	0.060	0.056	0.053	0.049	0.046	0.043	0.041
0.81	0.068	0.064	0.060	0.056	0.052	0.049	0.046	0.043	0.040	0.038
0.82	0.063	0.059	0.056	0.052	0.049	0.045	0.042	0.040	0.037	0.035
0.83	0.059	0.055	0.052	0.048	0.045	0.042	0.039	0.037	0.034	0.032
0.84	0.055	0.052	0.048	0.045	0.042	0.039	0.036	0.034	0.032	0.029
0.85	0.052	0.048	0.045	0.042	0.039	0.036	0.034	0.031	0.029	0.027
0.86	0.048	0.045	0.042	0.039	0.036	0.033	0.031	0.029	0.027	0.025
0.87	0.045	0.042	0.039	0.036	0.033	0.031	0.029	0.026	0.025	0.023
0.88	0.042	0.039	0.036	0.033	0.031	0.028	0.026	0.024	0.022	0.021
0.89	0.039	0.036	0.033	0.031	0.028	0.026	0.024	0.022	0.021	0.019
0.90	0.036	0.033	0.031	0.028	0.026	0.024	0.022	0.020	0.019	0.017
0.91	0.034	0.031	0.028	0.026	0.024	0.022	0.020	0.019	0.017	0.016
0.92	0.031	0.029	0.026	0.024	0.022	0.020	0.019	0.017	0.016	0.015
0.93	0.029	0.026	0.024	0.022	0.020	0.019	0.017	0.016	0.014	0.013
0.94	0.027	0.024	0.022	0.020	0.019	0.017	0.016	0.014	0.013	0.012
0.95	0.025	0.023	0.021	0.019	0.017	0.016	0.014	0.013	0.012	0.011
1.00	0.017	0.015	0.014	0.012	0.011	0.010	0.009	0.008	0.007	0.007
1.05	0.011	0.010	0.009	0.008	0.007	0.006	0.006	0.005	0.005	0.004
1.10	0.007	0.006	0.006	0.005	0.004	0.004	0.003	0.003	0.003	0.002
1.20	0.003	0.002	0.002	0.002	0.002	0.001	0.001	0.001	0.001	0.001
1.30	0.001	0.001	0.001	0.001	0.000	0.000	0.000	0.000	0.000	0.000

TABLE 5.2.2A (continued)

 $\exp(-B \sin^2 \theta/\lambda^2)$

$\frac{\sin \theta}{\lambda}$	$B=5.1$	5.2	5.3	5.4	5.5	5.6	5.7	5.8	5.9	6.0
0.01	0.999	0.999	0.999	0.999	0.999	0.999	0.999	0.999	0.999	0.999
0.02	0.998	0.998	0.998	0.998	0.998	0.998	0.998	0.998	0.998	0.998
0.03	0.995	0.995	0.995	0.995	0.995	0.995	0.995	0.995	0.995	0.995
0.04	0.992	0.992	0.992	0.991	0.991	0.991	0.991	0.991	0.991	0.990
0.05	0.987	0.987	0.987	0.987	0.986	0.986	0.986	0.986	0.985	0.985
0.06	0.982	0.981	0.981	0.981	0.980	0.980	0.980	0.979	0.979	0.979
0.07	0.975	0.975	0.974	0.974	0.973	0.973	0.972	0.972	0.972	0.971
0.08	0.968	0.967	0.967	0.966	0.965	0.965	0.964	0.964	0.963	0.962
0.09	0.960	0.959	0.958	0.957	0.956	0.956	0.955	0.954	0.953	0.953
0.10	0.950	0.949	0.948	0.947	0.946	0.946	0.945	0.944	0.943	0.942
0.11	0.940	0.939	0.938	0.937	0.936	0.934	0.933	0.932	0.931	0.930
0.12	0.929	0.928	0.927	0.925	0.924	0.923	0.921	0.920	0.919	0.917
0.13	0.917	0.916	0.914	0.913	0.911	0.910	0.908	0.907	0.905	0.904
0.14	0.905	0.903	0.901	0.900	0.898	0.896	0.894	0.893	0.891	0.889
0.15	0.892	0.890	0.888	0.886	0.884	0.882	0.880	0.878	0.876	0.874
0.16	0.878	0.875	0.873	0.871	0.869	0.866	0.864	0.862	0.860	0.858
0.17	0.863	0.860	0.858	0.856	0.853	0.851	0.848	0.846	0.843	0.841
0.18	0.848	0.845	0.842	0.839	0.837	0.834	0.831	0.829	0.826	0.823
0.19	0.832	0.829	0.826	0.823	0.820	0.817	0.814	0.811	0.808	0.805
0.20	0.815	0.812	0.809	0.806	0.803	0.799	0.796	0.793	0.790	0.787
0.21	0.799	0.795	0.792	0.788	0.785	0.781	0.778	0.774	0.771	0.768
0.22	0.781	0.777	0.774	0.770	0.766	0.763	0.759	0.755	0.752	0.748
0.23	0.764	0.760	0.756	0.752	0.748	0.744	0.740	0.736	0.732	0.728
0.24	0.745	0.741	0.737	0.733	0.728	0.724	0.720	0.716	0.712	0.708
0.25	0.727	0.723	0.718	0.714	0.709	0.705	0.700	0.696	0.692	0.687
0.26	0.708	0.704	0.699	0.694	0.689	0.685	0.680	0.676	0.671	0.667
0.27	0.689	0.684	0.680	0.675	0.670	0.665	0.660	0.655	0.650	0.646
0.28	0.670	0.665	0.660	0.655	0.650	0.645	0.640	0.635	0.630	0.625
0.29	0.651	0.646	0.640	0.635	0.630	0.624	0.619	0.614	0.609	0.604
0.30	0.632	0.626	0.621	0.615	0.610	0.604	0.599	0.593	0.588	0.583
0.31	0.613	0.607	0.601	0.595	0.589	0.584	0.578	0.573	0.567	0.562
0.32	0.593	0.587	0.581	0.575	0.569	0.564	0.558	0.552	0.547	0.541
0.33	0.574	0.568	0.561	0.555	0.549	0.543	0.538	0.532	0.526	0.520
0.34	0.555	0.548	0.542	0.536	0.530	0.523	0.517	0.511	0.506	0.500
0.35	0.535	0.529	0.522	0.516	0.510	0.504	0.497	0.491	0.485	0.480
0.36	0.516	0.510	0.503	0.497	0.490	0.484	0.478	0.472	0.466	0.460
0.37	0.497	0.491	0.484	0.477	0.471	0.465	0.458	0.452	0.446	0.440
0.38	0.479	0.472	0.465	0.459	0.452	0.445	0.439	0.433	0.427	0.420
0.39	0.460	0.453	0.447	0.440	0.433	0.427	0.420	0.414	0.408	0.401
0.40	0.442	0.435	0.428	0.421	0.415	0.408	0.402	0.395	0.389	0.383
0.41	0.424	0.417	0.410	0.403	0.397	0.390	0.384	0.377	0.371	0.365
0.42	0.407	0.400	0.393	0.386	0.379	0.372	0.366	0.359	0.353	0.347
0.43	0.389	0.382	0.375	0.368	0.362	0.355	0.349	0.342	0.336	0.330
0.44	0.373	0.365	0.358	0.352	0.345	0.338	0.332	0.325	0.319	0.313
0.45	0.356	0.349	0.342	0.335	0.328	0.322	0.315	0.309	0.303	0.297
0.46	0.340	0.333	0.326	0.319	0.312	0.306	0.299	0.293	0.287	0.281
0.47	0.324	0.317	0.310	0.303	0.297	0.290	0.284	0.278	0.272	0.266
0.48	0.309	0.302	0.295	0.288	0.282	0.275	0.269	0.263	0.257	0.251
0.49	0.294	0.287	0.280	0.273	0.267	0.261	0.254	0.248	0.243	0.237
0.50	0.279	0.273	0.266	0.259	0.253	0.247	0.241	0.235	0.229	0.223

TABLE 5.2.2A (continued)

 $\exp(-B \sin^2 \theta / \lambda^2)$

$\frac{\sin \theta}{\lambda}$	$B=5.1$	5.2	5.3	5.4	5.5	5.6	5.7	5.8	5.9	6.0
0.51	0.265	0.259	0.252	0.245	0.239	0.233	0.227	0.221	0.216	0.210
0.52	0.252	0.245	0.239	0.232	0.226	0.220	0.214	0.208	0.203	0.197
0.53	0.239	0.232	0.226	0.219	0.213	0.207	0.202	0.196	0.191	0.185
0.54	0.226	0.220	0.213	0.207	0.201	0.195	0.190	0.184	0.179	0.174
0.55	0.214	0.207	0.201	0.195	0.189	0.184	0.178	0.173	0.168	0.163
0.56	0.202	0.196	0.190	0.184	0.178	0.173	0.167	0.162	0.157	0.152
0.57	0.191	0.185	0.179	0.173	0.167	0.162	0.157	0.152	0.147	0.142
0.58	0.180	0.174	0.168	0.163	0.157	0.152	0.147	0.142	0.137	0.133
0.59	0.169	0.164	0.158	0.153	0.147	0.142	0.137	0.133	0.128	0.124
0.60	0.159	0.154	0.148	0.143	0.138	0.133	0.128	0.124	0.120	0.115
0.61	0.150	0.144	0.139	0.134	0.129	0.124	0.120	0.116	0.111	0.107
0.62	0.141	0.135	0.130	0.125	0.121	0.116	0.112	0.108	0.104	0.100
0.63	0.132	0.127	0.122	0.117	0.113	0.108	0.104	0.100	0.096	0.092
0.64	0.124	0.119	0.114	0.110	0.105	0.101	0.097	0.093	0.089	0.086
0.65	0.116	0.111	0.107	0.102	0.098	0.094	0.090	0.086	0.083	0.079
0.66	0.108	0.104	0.099	0.095	0.091	0.087	0.083	0.080	0.077	0.073
0.67	0.101	0.097	0.093	0.089	0.085	0.081	0.077	0.074	0.071	0.068
0.68	0.095	0.090	0.086	0.082	0.079	0.075	0.072	0.068	0.065	0.062
0.69	0.088	0.084	0.080	0.076	0.073	0.070	0.066	0.063	0.060	0.057
0.70	0.082	0.078	0.074	0.071	0.068	0.064	0.061	0.058	0.056	0.053
0.71	0.076	0.073	0.069	0.066	0.063	0.059	0.057	0.054	0.051	0.049
0.72	0.071	0.067	0.064	0.061	0.058	0.055	0.052	0.049	0.047	0.045
0.73	0.066	0.063	0.059	0.056	0.053	0.051	0.048	0.045	0.043	0.041
0.74	0.061	0.058	0.055	0.052	0.049	0.047	0.044	0.042	0.040	0.037
0.75	0.057	0.054	0.051	0.048	0.045	0.043	0.041	0.038	0.036	0.034
0.76	0.053	0.050	0.047	0.044	0.042	0.039	0.037	0.035	0.033	0.031
0.77	0.049	0.046	0.043	0.041	0.038	0.036	0.034	0.032	0.030	0.029
0.78	0.045	0.042	0.040	0.037	0.035	0.033	0.031	0.029	0.028	0.026
0.79	0.041	0.039	0.037	0.034	0.032	0.030	0.029	0.027	0.025	0.024
0.80	0.038	0.036	0.034	0.032	0.030	0.028	0.026	0.024	0.023	0.021
0.81	0.035	0.033	0.031	0.029	0.027	0.025	0.024	0.022	0.021	0.020
0.82	0.032	0.030	0.028	0.026	0.025	0.023	0.022	0.020	0.019	0.018
0.83	0.030	0.028	0.026	0.024	0.023	0.021	0.020	0.018	0.017	0.016
0.84	0.027	0.025	0.024	0.022	0.021	0.019	0.018	0.017	0.016	0.015
0.85	0.025	0.023	0.022	0.020	0.019	0.017	0.016	0.015	0.014	0.013
0.86	0.023	0.021	0.020	0.018	0.017	0.016	0.015	0.014	0.013	0.012
0.87	0.021	0.020	0.018	0.017	0.016	0.014	0.013	0.012	0.011	0.011
0.88	0.019	0.018	0.017	0.015	0.014	0.013	0.012	0.011	0.010	0.010
0.89	0.018	0.016	0.015	0.014	0.013	0.012	0.011	0.010	0.009	0.009
0.90	0.016	0.015	0.014	0.013	0.012	0.011	0.010	0.009	0.008	0.008
0.91	0.015	0.013	0.012	0.011	0.011	0.010	0.009	0.008	0.008	0.007
0.92	0.013	0.012	0.011	0.010	0.010	0.009	0.008	0.007	0.007	0.006
0.93	0.012	0.011	0.010	0.009	0.009	0.008	0.007	0.007	0.006	0.006
0.94	0.011	0.010	0.009	0.008	0.008	0.007	0.006	0.006	0.005	0.005
0.95	0.010	0.009	0.008	0.008	0.007	0.006	0.006	0.005	0.005	0.004
0.96	0.009	0.008	0.008	0.007	0.006	0.006	0.005	0.005	0.004	0.004
0.97	0.008	0.008	0.007	0.006	0.006	0.005	0.005	0.004	0.004	0.004
0.98	0.007	0.007	0.006	0.006	0.005	0.005	0.004	0.004	0.003	0.003
1.00	0.006	0.006	0.005	0.005	0.004	0.004	0.003	0.003	0.003	0.002
1.10	0.002	0.002	0.002	0.001	0.001	0.001	0.001	0.001	0.001	0.001

TABLE 5.2.2A (continued)

 $\exp(-B \sin^2 \theta/\lambda^2)$

$\frac{\sin \theta}{\lambda}$	$B=6.1$	6.2	6.3	6.4	6.5	6.6	6.7	6.8	6.9	7.0
0.01	0.999	0.999	0.999	0.999	0.999	0.999	0.999	0.999	0.999	0.999
0.02	0.998	0.998	0.997	0.997	0.997	0.997	0.997	0.997	0.997	0.997
0.03	0.995	0.994	0.994	0.994	0.994	0.994	0.994	0.994	0.994	0.994
0.04	0.990	0.990	0.990	0.990	0.990	0.989	0.989	0.989	0.989	0.989
0.05	0.985	0.985	0.984	0.984	0.984	0.984	0.983	0.983	0.983	0.983
0.06	0.978	0.978	0.978	0.977	0.977	0.977	0.976	0.976	0.975	0.975
0.07	0.971	0.970	0.970	0.969	0.969	0.968	0.968	0.967	0.967	0.966
0.08	0.962	0.961	0.960	0.960	0.959	0.959	0.958	0.957	0.957	0.956
0.09	0.952	0.951	0.950	0.949	0.949	0.948	0.947	0.946	0.946	0.945
0.10	0.941	0.940	0.939	0.938	0.937	0.936	0.935	0.934	0.933	0.932
0.11	0.929	0.928	0.927	0.925	0.924	0.923	0.922	0.921	0.920	0.919
0.12	0.916	0.915	0.913	0.912	0.911	0.909	0.908	0.907	0.905	0.904
0.13	0.902	0.901	0.899	0.897	0.896	0.894	0.893	0.891	0.890	0.888
0.14	0.887	0.886	0.884	0.882	0.880	0.879	0.877	0.875	0.874	0.872
0.15	0.872	0.870	0.868	0.866	0.864	0.862	0.860	0.858	0.856	0.854
0.16	0.855	0.853	0.851	0.849	0.847	0.845	0.842	0.840	0.838	0.836
0.17	0.838	0.836	0.834	0.831	0.829	0.826	0.824	0.822	0.819	0.817
0.18	0.821	0.818	0.815	0.813	0.810	0.807	0.805	0.802	0.800	0.797
0.19	0.802	0.799	0.797	0.794	0.791	0.788	0.785	0.782	0.780	0.777
0.20	0.783	0.780	0.777	0.774	0.771	0.768	0.765	0.762	0.759	0.756
0.21	0.764	0.761	0.757	0.754	0.751	0.747	0.744	0.741	0.738	0.734
0.22	0.744	0.741	0.737	0.734	0.730	0.727	0.723	0.720	0.716	0.713
0.23	0.724	0.720	0.717	0.713	0.709	0.705	0.702	0.698	0.694	0.691
0.24	0.704	0.700	0.696	0.692	0.688	0.684	0.680	0.676	0.672	0.668
0.25	0.683	0.679	0.675	0.670	0.666	0.662	0.658	0.654	0.650	0.646
0.26	0.662	0.658	0.653	0.649	0.644	0.640	0.636	0.631	0.627	0.623
0.27	0.641	0.636	0.632	0.627	0.623	0.618	0.614	0.609	0.605	0.600
0.28	0.620	0.615	0.610	0.605	0.601	0.596	0.591	0.587	0.582	0.578
0.29	0.599	0.594	0.589	0.584	0.579	0.574	0.569	0.564	0.560	0.555
0.30	0.578	0.572	0.567	0.562	0.557	0.552	0.547	0.542	0.537	0.533
0.31	0.556	0.551	0.546	0.541	0.535	0.530	0.525	0.520	0.515	0.510
0.32	0.535	0.530	0.525	0.519	0.514	0.509	0.504	0.498	0.493	0.488
0.33	0.515	0.509	0.504	0.498	0.493	0.487	0.482	0.477	0.472	0.467
0.34	0.494	0.488	0.483	0.477	0.472	0.466	0.461	0.456	0.450	0.445
0.35	0.474	0.468	0.462	0.457	0.451	0.446	0.440	0.435	0.429	0.424
0.36	0.454	0.448	0.442	0.436	0.431	0.425	0.420	0.414	0.409	0.404
0.37	0.434	0.428	0.422	0.416	0.411	0.405	0.400	0.394	0.389	0.384
0.38	0.414	0.408	0.403	0.397	0.391	0.386	0.380	0.375	0.369	0.364
0.39	0.395	0.389	0.384	0.378	0.372	0.366	0.361	0.355	0.350	0.345
0.40	0.377	0.371	0.365	0.359	0.353	0.348	0.342	0.337	0.332	0.326
0.41	0.359	0.353	0.347	0.341	0.335	0.330	0.324	0.319	0.314	0.308
0.42	0.341	0.335	0.329	0.323	0.318	0.312	0.307	0.301	0.296	0.291
0.43	0.324	0.318	0.312	0.306	0.301	0.295	0.290	0.284	0.279	0.274
0.44	0.307	0.301	0.295	0.290	0.284	0.279	0.273	0.268	0.263	0.258
0.45	0.291	0.285	0.279	0.274	0.268	0.263	0.257	0.252	0.247	0.242
0.46	0.275	0.269	0.264	0.258	0.253	0.247	0.242	0.237	0.232	0.227
0.47	0.260	0.254	0.249	0.243	0.238	0.233	0.228	0.223	0.218	0.213
0.48	0.245	0.240	0.234	0.229	0.224	0.219	0.214	0.209	0.204	0.199
0.49	0.231	0.226	0.220	0.215	0.210	0.205	0.200	0.195	0.191	0.186
0.50	0.218	0.212	0.207	0.202	0.197	0.192	0.187	0.183	0.178	0.174

TABLE 5.2.2A (continued)

$$\exp(-B \sin^2 \theta / \lambda^2)$$

$\frac{\sin \theta}{\lambda}$	$B=6.1$	6.2	6.3	6.4	6.5	6.6	6.7	6.8	6.9	7.0
0.51	0.205	0.199	0.194	0.189	0.184	0.180	0.175	0.171	0.166	0.162
0.52	0.192	0.187	0.182	0.177	0.172	0.168	0.163	0.159	0.155	0.151
0.53	0.180	0.175	0.170	0.166	0.161	0.157	0.152	0.148	0.144	0.140
0.54	0.169	0.164	0.159	0.155	0.150	0.146	0.142	0.138	0.134	0.130
0.55	0.158	0.153	0.149	0.144	0.140	0.136	0.132	0.128	0.124	0.120
0.56	0.148	0.143	0.139	0.134	0.130	0.126	0.122	0.119	0.115	0.111
0.57	0.138	0.133	0.129	0.125	0.121	0.117	0.113	0.110	0.106	0.103
0.58	0.128	0.124	0.120	0.116	0.112	0.109	0.105	0.102	0.098	0.095
0.59	0.120	0.116	0.112	0.108	0.104	0.101	0.097	0.094	0.091	0.087
0.60	0.111	0.107	0.104	0.100	0.096	0.093	0.090	0.086	0.083	0.080
0.61	0.103	0.100	0.096	0.092	0.089	0.086	0.083	0.080	0.077	0.074
0.62	0.096	0.092	0.089	0.085	0.082	0.079	0.076	0.073	0.070	0.068
0.63	0.089	0.085	0.082	0.079	0.076	0.073	0.070	0.067	0.065	0.062
0.64	0.082	0.079	0.076	0.073	0.070	0.067	0.064	0.062	0.059	0.057
0.65	0.076	0.073	0.070	0.067	0.064	0.062	0.059	0.057	0.054	0.052
0.66	0.070	0.067	0.064	0.062	0.059	0.056	0.054	0.052	0.050	0.047
0.67	0.065	0.062	0.059	0.057	0.054	0.052	0.049	0.047	0.045	0.043
0.68	0.060	0.057	0.054	0.052	0.050	0.047	0.045	0.043	0.041	0.039
0.69	0.055	0.052	0.050	0.047	0.045	0.043	0.041	0.039	0.037	0.036
0.70	0.050	0.048	0.046	0.043	0.041	0.039	0.038	0.036	0.034	0.032
0.71	0.046	0.044	0.042	0.040	0.038	0.036	0.034	0.032	0.031	0.029
0.72	0.042	0.040	0.038	0.036	0.034	0.033	0.031	0.029	0.028	0.027
0.73	0.039	0.037	0.035	0.033	0.031	0.030	0.028	0.027	0.025	0.024
0.74	0.035	0.034	0.032	0.030	0.028	0.027	0.026	0.024	0.023	0.022
0.75	0.032	0.031	0.029	0.027	0.026	0.024	0.023	0.022	0.021	0.019
0.76	0.030	0.028	0.026	0.025	0.023	0.022	0.021	0.020	0.019	0.018
0.77	0.027	0.025	0.024	0.022	0.021	0.020	0.019	0.018	0.017	0.016
0.78	0.024	0.023	0.022	0.020	0.019	0.018	0.017	0.016	0.015	0.014
0.79	0.022	0.021	0.020	0.018	0.017	0.016	0.015	0.014	0.013	0.013
0.80	0.020	0.019	0.018	0.017	0.016	0.015	0.014	0.013	0.012	0.011
0.81	0.018	0.017	0.016	0.015	0.014	0.013	0.012	0.012	0.011	0.010
0.82	0.017	0.015	0.014	0.014	0.013	0.012	0.011	0.010	0.010	0.009
0.83	0.015	0.014	0.013	0.012	0.011	0.011	0.010	0.009	0.009	0.008
0.84	0.014	0.013	0.012	0.011	0.010	0.009	0.009	0.008	0.008	0.007
0.85	0.012	0.011	0.011	0.010	0.009	0.008	0.008	0.007	0.007	0.006
0.86	0.011	0.010	0.009	0.009	0.008	0.008	0.007	0.007	0.006	0.006
0.87	0.010	0.009	0.008	0.008	0.007	0.007	0.006	0.006	0.005	0.005
0.88	0.009	0.008	0.008	0.007	0.007	0.006	0.006	0.005	0.005	0.004
0.89	0.008	0.007	0.007	0.006	0.006	0.005	0.005	0.005	0.004	0.004
0.90	0.007	0.007	0.006	0.006	0.005	0.005	0.004	0.004	0.004	0.003
0.91	0.006	0.006	0.005	0.005	0.005	0.004	0.004	0.004	0.003	0.003
0.92	0.006	0.005	0.005	0.004	0.004	0.004	0.003	0.003	0.003	0.003
0.93	0.005	0.005	0.004	0.004	0.004	0.003	0.003	0.003	0.003	0.002
0.94	0.005	0.004	0.004	0.003	0.003	0.003	0.003	0.002	0.002	0.002
0.95	0.004	0.004	0.003	0.003	0.003	0.003	0.002	0.002	0.002	0.002
0.96	0.004	0.003	0.003	0.003	0.003	0.002	0.002	0.002	0.002	0.002
0.97	0.003	0.003	0.003	0.002	0.002	0.002	0.002	0.002	0.002	0.001
0.98	0.003	0.003	0.002	0.002	0.002	0.002	0.002	0.001	0.001	0.001
0.99	0.003	0.002	0.002	0.002	0.002	0.002	0.001	0.001	0.001	0.001
1.00	0.002	0.002	0.002	0.002	0.002	0.001	0.001	0.001	0.001	0.001

TABLE 5.2.2A (continued)

 $\exp(-B \sin^2 \theta/\lambda^2)$

$\frac{\sin \theta}{\lambda}$	$B=7.1$	7.2	7.3	7.4	7.5	7.6	7.7	7.8	7.9	8.0
0.01	0.999	0.999	0.999	0.999	0.999	0.999	0.999	0.999	0.999	0.999
0.02	0.997	0.997	0.997	0.997	0.997	0.997	0.997	0.997	0.997	0.997
0.03	0.994	0.994	0.993	0.993	0.993	0.993	0.993	0.993	0.993	0.993
0.04	0.989	0.989	0.988	0.988	0.988	0.988	0.988	0.988	0.987	0.987
0.05	0.982	0.982	0.982	0.982	0.981	0.981	0.981	0.981	0.980	0.980
0.06	0.975	0.974	0.974	0.974	0.973	0.973	0.973	0.972	0.972	0.972
0.07	0.966	0.965	0.965	0.964	0.964	0.963	0.963	0.963	0.962	0.962
0.08	0.956	0.955	0.954	0.954	0.953	0.953	0.952	0.951	0.951	0.950
0.09	0.944	0.943	0.943	0.942	0.941	0.940	0.940	0.939	0.938	0.937
0.10	0.931	0.931	0.930	0.929	0.928	0.927	0.926	0.925	0.924	0.923
0.11	0.918	0.917	0.915	0.914	0.913	0.912	0.911	0.910	0.909	0.908
0.12	0.903	0.902	0.900	0.899	0.898	0.896	0.895	0.894	0.892	0.891
0.13	0.887	0.885	0.884	0.882	0.881	0.879	0.878	0.876	0.875	0.874
0.14	0.870	0.868	0.867	0.865	0.863	0.862	0.860	0.858	0.857	0.855
0.15	0.852	0.850	0.849	0.847	0.845	0.843	0.841	0.839	0.837	0.835
0.16	0.834	0.832	0.830	0.827	0.825	0.823	0.821	0.819	0.817	0.815
0.17	0.814	0.812	0.810	0.807	0.805	0.803	0.800	0.798	0.796	0.794
0.18	0.795	0.792	0.789	0.787	0.784	0.782	0.779	0.777	0.774	0.772
0.19	0.774	0.771	0.768	0.766	0.763	0.760	0.757	0.755	0.752	0.749
0.20	0.753	0.750	0.747	0.744	0.741	0.738	0.735	0.732	0.729	0.726
0.21	0.731	0.728	0.725	0.722	0.718	0.715	0.712	0.709	0.706	0.703
0.22	0.709	0.706	0.702	0.699	0.696	0.692	0.689	0.686	0.682	0.679
0.23	0.687	0.683	0.680	0.676	0.673	0.669	0.665	0.662	0.658	0.655
0.24	0.664	0.661	0.657	0.653	0.649	0.645	0.642	0.638	0.634	0.631
0.25	0.642	0.638	0.634	0.630	0.626	0.622	0.618	0.614	0.610	0.607
0.26	0.619	0.615	0.610	0.606	0.602	0.598	0.594	0.590	0.586	0.582
0.27	0.596	0.592	0.587	0.583	0.579	0.575	0.570	0.566	0.562	0.558
0.28	0.573	0.569	0.564	0.560	0.555	0.551	0.547	0.543	0.538	0.534
0.29	0.550	0.546	0.541	0.537	0.532	0.528	0.523	0.519	0.515	0.510
0.30	0.528	0.523	0.518	0.514	0.509	0.505	0.500	0.496	0.491	0.487
0.31	0.505	0.501	0.496	0.491	0.486	0.482	0.477	0.473	0.468	0.464
0.32	0.483	0.478	0.474	0.469	0.464	0.459	0.455	0.450	0.445	0.441
0.33	0.462	0.457	0.452	0.447	0.442	0.437	0.432	0.428	0.423	0.418
0.34	0.440	0.435	0.430	0.425	0.420	0.415	0.411	0.406	0.401	0.397
0.35	0.419	0.414	0.409	0.404	0.399	0.394	0.389	0.385	0.380	0.375
0.36	0.398	0.393	0.388	0.383	0.378	0.373	0.369	0.364	0.359	0.355
0.37	0.378	0.373	0.368	0.363	0.358	0.353	0.348	0.344	0.339	0.334
0.38	0.359	0.354	0.348	0.344	0.339	0.334	0.329	0.324	0.320	0.315
0.39	0.340	0.334	0.329	0.324	0.320	0.315	0.310	0.305	0.301	0.296
0.40	0.321	0.316	0.311	0.306	0.301	0.296	0.292	0.287	0.283	0.278
0.41	0.303	0.298	0.293	0.288	0.283	0.279	0.274	0.270	0.265	0.261
0.42	0.286	0.281	0.276	0.271	0.266	0.262	0.257	0.253	0.248	0.244
0.43	0.269	0.264	0.259	0.255	0.250	0.245	0.241	0.236	0.232	0.228
0.44	0.253	0.248	0.243	0.239	0.234	0.230	0.225	0.221	0.217	0.213
0.45	0.237	0.233	0.228	0.223	0.219	0.215	0.210	0.206	0.202	0.198
0.46	0.223	0.218	0.213	0.209	0.205	0.200	0.196	0.192	0.188	0.184
0.47	0.208	0.204	0.199	0.195	0.191	0.187	0.183	0.179	0.175	0.171
0.48	0.195	0.190	0.186	0.182	0.178	0.174	0.170	0.166	0.162	0.158
0.49	0.182	0.178	0.173	0.169	0.165	0.161	0.157	0.154	0.150	0.146
0.50	0.169	0.165	0.161	0.157	0.153	0.150	0.146	0.142	0.139	0.135

TABLE 5.2.2A (continued)

 $\exp(-B \sin^2 \theta / \lambda^2)$

$\frac{\sin \theta}{\lambda}$	$B=7.1$	7.2	7.3	7.4	7.5	7.6	7.7	7.8	7.9	8.0
0.51	0.158	0.154	0.150	0.146	0.142	0.139	0.135	0.131	0.128	0.125
0.52	0.147	0.143	0.139	0.135	0.132	0.128	0.125	0.121	0.118	0.115
0.53	0.136	0.132	0.129	0.125	0.122	0.118	0.115	0.112	0.109	0.106
0.54	0.126	0.123	0.119	0.116	0.112	0.109	0.106	0.103	0.100	0.097
0.55	0.117	0.113	0.110	0.107	0.103	0.100	0.097	0.094	0.092	0.089
0.56	0.108	0.105	0.101	0.098	0.095	0.092	0.089	0.087	0.084	0.081
0.57	0.100	0.096	0.093	0.090	0.087	0.085	0.082	0.079	0.077	0.074
0.58	0.092	0.089	0.086	0.083	0.080	0.078	0.075	0.073	0.070	0.068
0.59	0.084	0.082	0.079	0.076	0.073	0.071	0.069	0.066	0.064	0.062
0.60	0.078	0.075	0.072	0.070	0.067	0.065	0.063	0.060	0.058	0.056
0.61	0.071	0.069	0.066	0.064	0.061	0.059	0.057	0.055	0.053	0.051
0.62	0.065	0.063	0.060	0.058	0.056	0.054	0.052	0.050	0.048	0.046
0.63	0.060	0.057	0.055	0.053	0.051	0.049	0.047	0.045	0.043	0.042
0.64	0.055	0.052	0.050	0.048	0.046	0.044	0.043	0.041	0.039	0.038
0.65	0.050	0.048	0.046	0.044	0.042	0.040	0.039	0.037	0.036	0.034
0.66	0.045	0.043	0.042	0.040	0.038	0.036	0.035	0.033	0.032	0.031
0.67	0.041	0.039	0.038	0.036	0.035	0.033	0.032	0.030	0.029	0.028
0.68	0.038	0.036	0.034	0.033	0.031	0.030	0.028	0.027	0.026	0.025
0.69	0.034	0.032	0.031	0.030	0.028	0.027	0.026	0.024	0.023	0.022
0.70	0.031	0.029	0.028	0.027	0.025	0.024	0.023	0.022	0.021	0.020
0.71	0.028	0.027	0.025	0.024	0.023	0.022	0.021	0.020	0.019	0.018
0.72	0.025	0.024	0.023	0.022	0.020	0.019	0.018	0.018	0.017	0.016
0.73	0.023	0.022	0.020	0.019	0.018	0.017	0.017	0.016	0.015	0.014
0.74	0.020	0.019	0.018	0.017	0.016	0.016	0.015	0.014	0.013	0.013
0.75	0.018	0.017	0.016	0.016	0.015	0.014	0.013	0.012	0.012	0.011
0.76	0.017	0.016	0.015	0.014	0.013	0.012	0.012	0.011	0.010	0.010
0.77	0.015	0.014	0.013	0.012	0.012	0.011	0.010	0.010	0.009	0.009
0.78	0.013	0.013	0.012	0.011	0.010	0.010	0.009	0.009	0.008	0.008
0.79	0.012	0.011	0.011	0.010	0.009	0.009	0.008	0.008	0.007	0.007
0.80	0.011	0.010	0.009	0.009	0.008	0.008	0.007	0.007	0.006	0.006
0.81	0.009	0.009	0.008	0.008	0.007	0.007	0.006	0.006	0.006	0.005
0.82	0.008	0.008	0.007	0.007	0.006	0.006	0.006	0.005	0.005	0.005
0.83	0.008	0.007	0.007	0.006	0.006	0.005	0.005	0.005	0.004	0.004
0.84	0.007	0.006	0.006	0.005	0.005	0.005	0.004	0.004	0.004	0.004
0.85	0.006	0.006	0.005	0.005	0.004	0.004	0.004	0.004	0.003	0.003
0.90	0.003	0.003	0.003	0.002	0.002	0.002	0.002	0.002	0.002	0.002
0.95	0.002	0.002	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001
1.00	0.001	0.001	0.001	0.001	0.001	0.001	0.000	0.000	0.000	0.000

TABLE 5.2.2A (continued)

 $\exp(-B \sin^2 \theta/\lambda^2)$

$\frac{\sin \theta}{\lambda}$	$B=8.1$	8.2	8.3	8.4	8.5	8.6	8.7	8.8	8.9	9.0
0.01	0.999	0.999	0.999	0.999	0.999	0.999	0.999	0.999	0.999	0.999
0.02	0.997	0.997	0.997	0.997	0.997	0.997	0.997	0.996	0.996	0.996
0.03	0.993	0.993	0.993	0.992	0.992	0.992	0.992	0.992	0.992	0.992
0.04	0.987	0.987	0.987	0.987	0.986	0.986	0.986	0.986	0.986	0.986
0.05	0.980	0.980	0.979	0.979	0.979	0.979	0.978	0.978	0.978	0.978
0.06	0.971	0.971	0.971	0.970	0.970	0.970	0.969	0.969	0.968	0.968
0.07	0.961	0.961	0.960	0.960	0.959	0.959	0.958	0.958	0.957	0.957
0.08	0.949	0.949	0.948	0.948	0.947	0.946	0.946	0.945	0.945	0.944
0.09	0.936	0.936	0.935	0.934	0.933	0.933	0.932	0.931	0.930	0.930
0.10	0.922	0.921	0.920	0.919	0.919	0.918	0.917	0.916	0.915	0.914
0.11	0.907	0.906	0.904	0.903	0.902	0.901	0.900	0.899	0.898	0.897
0.12	0.890	0.889	0.887	0.886	0.885	0.884	0.882	0.881	0.880	0.878
0.13	0.872	0.871	0.869	0.868	0.866	0.865	0.863	0.862	0.860	0.859
0.14	0.853	0.852	0.850	0.848	0.847	0.845	0.843	0.842	0.840	0.838
0.15	0.833	0.832	0.830	0.828	0.826	0.824	0.822	0.820	0.819	0.817
0.16	0.813	0.811	0.809	0.807	0.804	0.802	0.800	0.798	0.796	0.794
0.17	0.791	0.789	0.787	0.784	0.782	0.780	0.778	0.775	0.773	0.771
0.18	0.769	0.767	0.764	0.762	0.759	0.757	0.754	0.752	0.749	0.747
0.19	0.746	0.744	0.741	0.738	0.736	0.733	0.730	0.728	0.725	0.723
0.20	0.723	0.720	0.717	0.715	0.712	0.709	0.706	0.703	0.700	0.698
0.21	0.700	0.697	0.693	0.690	0.687	0.684	0.681	0.678	0.675	0.672
0.22	0.676	0.672	0.669	0.666	0.663	0.660	0.656	0.653	0.650	0.647
0.23	0.651	0.648	0.645	0.641	0.638	0.634	0.631	0.628	0.624	0.621
0.24	0.627	0.624	0.620	0.616	0.613	0.609	0.606	0.602	0.599	0.595
0.25	0.603	0.599	0.595	0.592	0.588	0.584	0.581	0.577	0.573	0.570
0.26	0.578	0.574	0.571	0.567	0.563	0.559	0.555	0.552	0.548	0.544
0.27	0.554	0.550	0.546	0.542	0.538	0.534	0.530	0.526	0.523	0.519
0.28	0.530	0.526	0.522	0.518	0.514	0.510	0.506	0.502	0.498	0.494
0.29	0.506	0.502	0.498	0.493	0.489	0.485	0.481	0.477	0.473	0.469
0.30	0.482	0.478	0.474	0.470	0.465	0.461	0.457	0.453	0.449	0.445
0.31	0.459	0.455	0.450	0.446	0.442	0.438	0.433	0.429	0.425	0.421
0.32	0.436	0.432	0.427	0.423	0.419	0.415	0.410	0.406	0.402	0.398
0.33	0.414	0.409	0.405	0.401	0.396	0.392	0.388	0.384	0.379	0.375
0.34	0.392	0.388	0.383	0.379	0.374	0.370	0.366	0.362	0.357	0.353
0.35	0.371	0.366	0.362	0.357	0.353	0.349	0.344	0.340	0.336	0.332
0.36	0.350	0.346	0.341	0.337	0.332	0.328	0.324	0.320	0.316	0.311
0.37	0.330	0.325	0.321	0.317	0.312	0.308	0.304	0.300	0.296	0.292
0.38	0.310	0.306	0.302	0.297	0.293	0.289	0.285	0.281	0.277	0.273
0.39	0.292	0.287	0.283	0.279	0.274	0.270	0.266	0.262	0.258	0.254
0.40	0.274	0.269	0.265	0.261	0.257	0.253	0.249	0.245	0.241	0.237
0.41	0.256	0.252	0.248	0.244	0.240	0.236	0.232	0.228	0.224	0.220
0.42	0.240	0.235	0.231	0.227	0.223	0.219	0.216	0.212	0.208	0.204
0.43	0.224	0.220	0.216	0.212	0.208	0.204	0.200	0.196	0.193	0.189
0.44	0.208	0.204	0.201	0.197	0.193	0.189	0.186	0.182	0.179	0.175
0.45	0.194	0.190	0.186	0.183	0.179	0.175	0.172	0.168	0.165	0.162
0.46	0.180	0.176	0.173	0.169	0.166	0.162	0.159	0.155	0.152	0.149
0.47	0.167	0.163	0.160	0.156	0.153	0.150	0.146	0.143	0.140	0.137
0.48	0.155	0.151	0.148	0.144	0.141	0.138	0.135	0.132	0.129	0.126
0.49	0.143	0.140	0.136	0.133	0.130	0.127	0.124	0.121	0.118	0.115
0.50	0.132	0.129	0.126	0.122	0.119	0.116	0.114	0.111	0.108	0.105

TABLE 5.2.2A (continued)

$$\exp(-B \sin^2 \theta / \lambda^2)$$

$\frac{\sin \theta}{\lambda}$	$B=8.1$	8.2	8.3	8.4	8.5	8.6	8.7	8.8	8.9	9.0
0.51	0.122	0.119	0.115	0.112	0.110	0.107	0.104	0.101	0.099	0.096
0.52	0.112	0.109	0.106	0.103	0.100	0.098	0.095	0.093	0.090	0.088
0.53	0.103	0.100	0.097	0.094	0.092	0.089	0.087	0.084	0.082	0.080
0.54	0.094	0.092	0.089	0.086	0.084	0.081	0.079	0.077	0.075	0.072
0.55	0.086	0.084	0.081	0.079	0.076	0.074	0.072	0.070	0.068	0.066
0.56	0.079	0.076	0.074	0.072	0.070	0.067	0.065	0.063	0.061	0.059
0.57	0.072	0.070	0.067	0.065	0.063	0.061	0.059	0.057	0.055	0.054
0.58	0.066	0.063	0.061	0.059	0.057	0.055	0.054	0.052	0.050	0.048
0.59	0.060	0.058	0.056	0.054	0.052	0.050	0.048	0.047	0.045	0.044
0.60	0.054	0.052	0.050	0.049	0.047	0.045	0.044	0.042	0.041	0.039
0.61	0.049	0.047	0.046	0.044	0.042	0.041	0.039	0.038	0.036	0.035
0.62	0.044	0.043	0.041	0.040	0.038	0.037	0.035	0.034	0.033	0.031
0.63	0.040	0.039	0.037	0.036	0.034	0.033	0.032	0.030	0.029	0.028
0.64	0.036	0.035	0.033	0.032	0.031	0.030	0.028	0.027	0.026	0.025
0.65	0.033	0.031	0.030	0.029	0.028	0.026	0.025	0.024	0.023	0.022
0.66	0.029	0.028	0.027	0.026	0.025	0.024	0.023	0.022	0.021	0.020
0.67	0.026	0.025	0.024	0.023	0.022	0.021	0.020	0.019	0.018	0.018
0.68	0.024	0.023	0.022	0.021	0.020	0.019	0.018	0.017	0.016	0.016
0.69	0.021	0.020	0.019	0.018	0.017	0.017	0.016	0.015	0.014	0.014
0.70	0.019	0.018	0.017	0.016	0.016	0.015	0.014	0.013	0.013	0.012
0.71	0.017	0.016	0.015	0.014	0.014	0.013	0.012	0.012	0.011	0.011
0.72	0.015	0.014	0.014	0.013	0.012	0.012	0.011	0.010	0.010	0.009
0.73	0.013	0.013	0.012	0.011	0.011	0.010	0.010	0.009	0.009	0.008
0.74	0.012	0.011	0.011	0.010	0.010	0.009	0.009	0.008	0.008	0.007
0.75	0.011	0.010	0.009	0.009	0.008	0.008	0.007	0.007	0.007	0.006
0.76	0.009	0.009	0.008	0.008	0.007	0.007	0.007	0.006	0.006	0.006
0.77	0.008	0.008	0.007	0.007	0.006	0.006	0.006	0.005	0.005	0.005
0.78	0.007	0.007	0.006	0.006	0.006	0.005	0.005	0.005	0.004	0.004
0.79	0.006	0.006	0.006	0.005	0.005	0.005	0.004	0.004	0.004	0.004
0.80	0.006	0.005	0.005	0.005	0.004	0.004	0.004	0.004	0.003	0.003
0.85	0.003	0.003	0.002	0.002	0.002	0.002	0.002	0.002	0.002	0.001
0.90	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001

TABLE 5.2.2A (continued)

$$\exp(-B \sin^2 \theta / \lambda^2)$$

$\frac{\sin \theta}{\lambda}$	$B=9.1$	9.2	9.3	9.4	9.5	9.6	9.7	9.8	9.9	10.0
0.01	0.999	0.999	0.999	0.999	0.999	0.999	0.999	0.999	0.999	0.999
0.02	0.996	0.996	0.996	0.996	0.996	0.996	0.996	0.996	0.996	0.996
0.03	0.992	0.992	0.992	0.992	0.991	0.991	0.991	0.991	0.991	0.991
0.04	0.986	0.985	0.985	0.985	0.985	0.985	0.985	0.984	0.984	0.984
0.05	0.978	0.977	0.977	0.977	0.977	0.976	0.976	0.976	0.976	0.975
0.06	0.968	0.967	0.967	0.967	0.966	0.966	0.966	0.965	0.965	0.965
0.07	0.956	0.956	0.955	0.955	0.955	0.954	0.954	0.953	0.953	0.952
0.08	0.943	0.943	0.942	0.942	0.941	0.940	0.940	0.939	0.939	0.938
0.09	0.929	0.928	0.927	0.927	0.926	0.925	0.924	0.924	0.923	0.922
0.10	0.913	0.912	0.911	0.910	0.909	0.908	0.908	0.907	0.906	0.905
0.11	0.896	0.895	0.894	0.892	0.891	0.890	0.889	0.888	0.887	0.886
0.12	0.877	0.876	0.875	0.873	0.872	0.871	0.870	0.868	0.867	0.866
0.13	0.857	0.856	0.855	0.853	0.852	0.850	0.849	0.847	0.846	0.845
0.14	0.837	0.835	0.833	0.832	0.830	0.828	0.827	0.825	0.824	0.822
0.15	0.815	0.813	0.811	0.809	0.808	0.806	0.804	0.802	0.800	0.799
0.16	0.792	0.790	0.788	0.786	0.784	0.782	0.780	0.778	0.776	0.774
0.17	0.769	0.767	0.764	0.762	0.760	0.758	0.756	0.753	0.751	0.749
0.18	0.745	0.742	0.740	0.737	0.735	0.733	0.730	0.728	0.726	0.723
0.19	0.720	0.717	0.715	0.712	0.710	0.707	0.705	0.702	0.699	0.697
0.20	0.695	0.692	0.689	0.687	0.684	0.681	0.678	0.676	0.673	0.670
0.21	0.669	0.666	0.664	0.661	0.658	0.655	0.652	0.649	0.646	0.643
0.22	0.644	0.641	0.638	0.634	0.631	0.628	0.625	0.622	0.619	0.616
0.23	0.618	0.615	0.611	0.608	0.605	0.602	0.599	0.595	0.592	0.589
0.24	0.592	0.589	0.585	0.582	0.579	0.575	0.572	0.569	0.565	0.562
0.25	0.566	0.563	0.559	0.556	0.552	0.549	0.545	0.542	0.539	0.535
0.26	0.541	0.537	0.533	0.530	0.526	0.523	0.519	0.516	0.512	0.509
0.27	0.515	0.511	0.508	0.504	0.500	0.497	0.493	0.489	0.486	0.482
0.28	0.490	0.486	0.482	0.479	0.475	0.471	0.467	0.464	0.460	0.457
0.29	0.465	0.461	0.457	0.454	0.450	0.446	0.442	0.439	0.435	0.431
0.30	0.441	0.437	0.433	0.429	0.425	0.421	0.418	0.414	0.410	0.407
0.31	0.417	0.413	0.409	0.405	0.401	0.398	0.394	0.390	0.386	0.383
0.32	0.394	0.390	0.386	0.382	0.378	0.374	0.370	0.367	0.363	0.359
0.33	0.371	0.367	0.363	0.359	0.355	0.352	0.348	0.344	0.340	0.337
0.34	0.349	0.345	0.341	0.337	0.333	0.330	0.326	0.322	0.318	0.315
0.35	0.328	0.324	0.320	0.316	0.312	0.309	0.305	0.301	0.297	0.294
0.36	0.307	0.304	0.300	0.296	0.292	0.288	0.284	0.281	0.277	0.274
0.37	0.288	0.284	0.280	0.276	0.272	0.269	0.265	0.261	0.258	0.254
0.38	0.269	0.265	0.261	0.257	0.254	0.250	0.246	0.243	0.239	0.236
0.39	0.251	0.247	0.243	0.239	0.236	0.232	0.229	0.225	0.222	0.218
0.40	0.233	0.229	0.226	0.222	0.219	0.215	0.212	0.208	0.205	0.202
0.41	0.217	0.213	0.209	0.206	0.203	0.199	0.196	0.193	0.189	0.186
0.42	0.201	0.197	0.194	0.190	0.187	0.184	0.181	0.178	0.174	0.171
0.43	0.186	0.182	0.179	0.176	0.173	0.169	0.166	0.163	0.160	0.157
0.44	0.172	0.168	0.165	0.162	0.159	0.156	0.153	0.150	0.147	0.144
0.45	0.158	0.155	0.152	0.149	0.146	0.143	0.140	0.137	0.135	0.132
0.46	0.146	0.143	0.140	0.137	0.134	0.131	0.128	0.126	0.123	0.121
0.47	0.134	0.131	0.128	0.125	0.123	0.120	0.117	0.115	0.112	0.110
0.48	0.123	0.120	0.117	0.115	0.112	0.110	0.107	0.105	0.102	0.100
0.49	0.112	0.110	0.107	0.105	0.102	0.100	0.097	0.095	0.093	0.091
0.50	0.103	0.100	0.098	0.095	0.093	0.091	0.088	0.086	0.084	0.082

5.2. INTENSITY OF RADIATION DIFFRACTED BY A CRYSTAL

TABLE 5.2.2A (*continued*) $\exp(-B \sin^2 \theta/\lambda^2)$

$\frac{\sin \theta}{\lambda}$	$B=9.1$	9.2	9.3	9.4	9.5	9.6	9.7	9.8	9.9	10.0
0.51	0.094	0.091	0.089	0.087	0.085	0.082	0.080	0.078	0.076	0.074
0.52	0.085	0.083	0.081	0.079	0.077	0.075	0.073	0.071	0.069	0.067
0.53	0.078	0.075	0.073	0.071	0.069	0.067	0.066	0.064	0.062	0.060
0.54	0.070	0.068	0.066	0.065	0.063	0.061	0.059	0.057	0.056	0.054
0.55	0.064	0.062	0.060	0.058	0.056	0.055	0.053	0.052	0.050	0.049
0.56	0.058	0.056	0.054	0.052	0.051	0.049	0.048	0.046	0.045	0.043
0.57	0.052	0.050	0.049	0.047	0.046	0.044	0.043	0.041	0.040	0.039
0.58	0.047	0.045	0.044	0.042	0.041	0.040	0.038	0.037	0.036	0.035
0.59	0.042	0.041	0.039	0.038	0.037	0.035	0.034	0.033	0.032	0.031
0.60	0.038	0.036	0.035	0.034	0.033	0.032	0.030	0.029	0.028	0.027
0.61	0.034	0.033	0.031	0.030	0.029	0.028	0.027	0.026	0.025	0.024
0.62	0.030	0.029	0.028	0.027	0.026	0.025	0.024	0.023	0.022	0.021
0.63	0.027	0.026	0.025	0.024	0.023	0.022	0.021	0.020	0.020	0.019
0.64	0.024	0.023	0.022	0.021	0.020	0.020	0.019	0.018	0.017	0.017
0.65	0.021	0.021	0.020	0.019	0.018	0.017	0.017	0.016	0.015	0.015
0.66	0.019	0.018	0.017	0.017	0.016	0.015	0.015	0.014	0.013	0.013
0.67	0.017	0.016	0.015	0.015	0.014	0.013	0.013	0.012	0.012	0.011
0.68	0.015	0.014	0.014	0.013	0.012	0.012	0.011	0.011	0.010	0.010
0.69	0.013	0.013	0.012	0.011	0.011	0.010	0.010	0.009	0.009	0.009
0.70	0.012	0.011	0.010	0.010	0.010	0.009	0.009	0.008	0.008	0.007
0.71	0.010	0.010	0.009	0.009	0.008	0.008	0.008	0.007	0.007	0.006
0.72	0.009	0.008	0.008	0.008	0.007	0.007	0.007	0.006	0.006	0.006
0.73	0.008	0.007	0.007	0.007	0.006	0.006	0.006	0.005	0.005	0.005
0.74	0.007	0.006	0.006	0.006	0.006	0.005	0.005	0.005	0.004	0.004
0.75	0.006	0.006	0.005	0.005	0.005	0.005	0.004	0.004	0.004	0.004
0.80	0.003	0.003	0.003	0.002	0.002	0.002	0.002	0.002	0.002	0.002
0.90	0.001	0.001	0.001	0.000	0.000	0.000	0.000	0.000	0.000	0.000

TABLE 5.2.2B

Values of $\phi(x) = \frac{1}{x} \int_0^x \frac{\xi}{e^\xi - 1} d\xi$ as a Function of x

x	.0	.1	.2	.3	.4	.5	.6	.7	.8	.9
0	1.000	0.975	0.951	0.928	0.904	0.882	0.860	0.839	0.818	0.797
1	0.778	0.758	0.739	0.721	0.703	0.686	0.669	0.653	0.637	0.622
2	0.607	0.592	0.578	0.565	0.552	0.539	0.526	0.514	0.503	0.491
3	0.480	0.470	0.460	0.450	0.440	0.431	0.422	0.413	0.404	0.396
4	0.388	0.380	0.373	0.366	0.359	0.352	0.345	0.339	0.333	0.327
5	0.321	0.315	0.310	0.304	0.299	0.294	0.289	0.285	0.280	0.276
6	0.271	0.267	0.263	0.259	0.255	0.251	0.248	0.244	0.241	0.237

For $x \geq 7$, $\phi(x)$ is given to a sufficiently close approximation by the expression $1.642/x$. The values of $\phi(x)$ at integral values of x up to 20 are as follows:

x	7	8	9	10	11	12	13	14	15	16	17	18	19	20
$\phi(x)$	0.234	0.205	0.183	0.164	0.150	0.137	0.127	0.117	0.110	0.103	0.097	0.091	0.087	0.082

(Continued from page 241)

In general, however, B must be treated as an empirical constant, derived either by Wilson's method [19] or by the comparison of observed intensities with those calculated by successive refinement from an approximate structure. Typical values of B will be found in Volume III.

5.2.3. Integrated Reflection

(a) *Integrated Reflection from a Crystal Element*; to be used when crystal or polycrystalline specimen is bathed in a beam.

The structure amplitude $|F|$ does not define the amplitude of the radiation scattered in a particular direction when the crystal is set in a particular orientation; this amplitude depends upon a number of incidental factors, such as the perfection of the crystal. A more significant quantity is obtained by considering the power (energy per second) of the diffracted beam as the crystal is rotated through the reflecting position, starting and finishing in orientations for which no appreciable scattering occurs. The *integrated reflection* is then defined as

$$\rho = \int_{\theta_0 - \epsilon}^{\theta_0 + \epsilon} R(\theta) d\theta \quad \dots (10)$$

where $R(\theta)$ is the ratio of the *power* of the diffracted beam to the incident *intensity*, when the rays are incident at an angle θ with the reflecting planes. The angle θ_0 is the angle of maximum diffracted power, and ϵ is chosen to include effectively all the diffracted radiation.

An alternative definition of the integrated reflection is as follows. Let the crystal be turned with angular velocity ω about an axis parallel to the reflecting planes. As it passes through a small angular range in the neighbourhood of the reflecting angle θ_0 , a total amount of energy E is reflected. Then the integrated reflection is defined as $E\omega/I_0$.

If an infinitesimally small block δV of crystal reflects X-rays, it can be shown that the integrated reflection ρ is proportional to δV .

$$\rho = Q\delta V \quad \dots (11a)$$

$$\text{and } Q = \frac{1}{\sin 2\theta} \left(\frac{N e^2 |F|}{m c^2} \right)^2 \lambda^3 \frac{1 + \cos^2 2\theta}{2} \quad \dots (11b)$$

The quantity $1/\sin 2\theta$ is known as the Lorentz factor and the final term is the polarization factor (Table

5.1.2). Under any ordinary conditions the quantity $N^2 e^4 \lambda^3 / m^2 c^4$ can be treated as a constant.

Note that the integrated reflection ρ is proportional to the volume of the reflecting crystal or crystal element and has the *dimensions* of cm^2 . It is, however, independent of the shape of the crystal or crystal element.

(b) *Integrated Reflection from an Extended Crystal Face*; to be used when crystal or polycrystalline block is large enough to intercept the entire incident beam.

A different quantity, ρ' , also termed integrated reflection, is more appropriate for measuring diffracted beams from a large crystal face or from a large block of crystalline powder. Its definition is

$$\rho' = \int_{\theta_0 - \epsilon}^{\theta_0 + \epsilon} R'(\theta) d\theta = \frac{E\omega}{I} \quad \dots (12)$$

In this case $R'(\theta)$ is the ratio of the *power* of the reflected beam, at angle θ , to the *power* of the incident beam.

Note that ρ' is a *dimensionless* quantity that is characteristic of the crystal and the wavelength employed.

5.2.4. Correction of Intensities for Angle Factors

Although equations 5.2.3 (11) and (12) are the basic ones, they have to be adapted to the type of specimen used and to the experimental conditions, which may introduce a different form for the Lorentz factor. The following are some of the important cases:

5.2.4.1. SINGLE CRYSTAL: BEAM NORMAL TO ROTATION AXIS

(Oscillation and rotation photographs; normal incidence Weissenberg photographs.)

$$\rho \propto \frac{1 + \cos^2 2\theta}{\sin 2\theta} \frac{\cos \theta}{(\cos^2 \phi - \sin^2 \theta)^{\frac{1}{2}}} A(hkl) p' |F|^2 \quad \dots (13)$$

where ϕ is the angle between the axis of rotation and the reflecting planes, $A(hkl)$ is a transmission factor, and p' is the multiplicity, that is, the number of superimposed reflections.

If ϕ is zero, as for zero-layer lines on oscillation, rotation and Weissenberg photographs, the expression reduces to

$$\rho \propto \frac{1 + \cos^2 2\theta}{\sin 2\theta} A(hkl) p' |F|^2 \quad \dots (14)$$

5.2. INTENSITY OF RADIATION DIFFRACTED BY A CRYSTAL

5.2.4.2. SINGLE CRYSTAL: EQUI-INCLINATION WEISSENBERG PHOTOGRAPH

$$\rho \propto \frac{1 + \cos^2 2\theta}{\xi \cos \theta} A(hkl) |F|^2 \quad \dots (15)$$

where ξ is the usual cylindrical co-ordinate of the reciprocal-lattice point.

5.2.4.3. DEBYE-SCHERRER LINES ON CYLINDRICAL FILM

$$\rho \propto \frac{1 + \cos^2 2\theta}{\sin^2 \theta \cos \theta} A(\theta) p'' |F|^2 \quad \dots (16)$$

where p'' is the multiplicity, or number of superimposed reflections, appropriate to this method.

5.2.5. Lorentz-polarization Factors

Let us put the equation for the integrated reflection from a small crystal of volume V in the form

$$\rho \propto V L p |F|^2$$

where L is the Lorentz factor (Section 5.2.3) and p is the polarization factor (Section 5.1.2).

The Lorentz factor depends on the way in which P_λ , the reciprocal-lattice point $(hkl)_\lambda$, passes through the reflecting sphere. For a given experimental arrangement, the component v_n of the velocity of P_λ normal to the surface of the sphere will be proportional to the angular velocity ω . The ratio ω/v_n gives L . In the particular case where the axis of rotation is perpendicular to the plane containing the incident and reflected beams, $L^{-1} = \sin 2\theta$ (Section 5.2.3). As the Lorentz factor L and the polarization factor p always occur together, it is in practice convenient to be able to correct for them simultaneously. The function $(1 + \cos^2 2\theta)/\sin 2\theta$ is tabulated in Table 5.2.5A. This is the form of Lp appropriate to *zero-layer* reflections when the apparatus is set up to make oscillation, rotation or Weissenberg recordings. The same factor applies to reflections from planes parallel to the surface of an extended, infinitely thick crystal plate (cf. Section 5.3.1).

The intensity of Debye-Scherrer lines on a cylindrical film depends on $(1 + \cos^2 2\theta)/\sin^2 \theta \cos \theta$, the function which is tabulated in Table 5.2.5B. A still different factor, $(1 + \cos^2 2\theta)/\sin \theta \cos^2 \theta$, applies to reflection through an infinitely thin, extended crystal plate from a set of planes normal to its surface (cf. Section 5.3.3). This function is tabulated in Table 5.2.5C.

For a single crystal, in the more general case where the axis of rotation makes an angle $(\pi/2) - \mu$ with the incident X-ray beam and the reciprocal-lattice point P is on the n -layer (this layer being perpendicular to the axis of rotation), it may be shown that

$$L^{-1} = \cos \mu \cos \nu \sin Y \quad \dots (17)$$

The semi-angle of the cone of diffraction for n -layer reflections is $(\pi/2) - \nu$, and Y is the projection on the zero layer of the angle 2θ between incident and reflected beams. For each experimental arrangement L can also be expressed as a function of ξ and ζ , the radial and axial cylindrical co-ordinates of P . The following are the most generally used arrangements for the photography of the reciprocal lattice.

5.2.5.1. NORMAL-BEAM METHOD, $\mu=0$ (Section 4.4.1(a))

There are three equivalent expressions for L .

$$\left. \begin{aligned} L^{-1} &= \cos \nu \sin Y \\ L^{-1} &= \sin 2\theta \frac{(\cos^2 \phi - \sin^2 \theta)^{\frac{1}{2}}}{\cos \theta} \\ \text{and } L^{-1} &= (\sin^2 2\theta - \zeta^2)^{\frac{1}{2}} \end{aligned} \right\} \quad \dots (18)$$

The angle ϕ is that between the axis of rotation and the reflecting plane.

Buerger and Klein [3] point out that for an n -level Weissenberg photograph, $\cos \nu$ is constant and Y can immediately be found from the location of the diffraction spot on the film. Their paper includes a table of $L = \text{cosec } Y$ as a function of Y .

Cox and Shaw [6] have published a chart which, when drawn to scale and superimposed on a rotation photograph, enables $(\cos^2 \phi - \sin^2 \theta)^{\frac{1}{2}}/\cos \theta$ to be read off for each reflection.

Kaan and Cole [11] have constructed a similar but more convenient chart for rotation photographs which gives the value of the combined factor $(Lp)^{-1}$ for each reflection. The necessary data for the construction of this chart are given in Table 5.2.5D.

Cochran [5] has expressed the combined factor $(Lp)^{-1}$ as a function of ξ and ζ and gives a chart which can be used in conjunction with a drawing of a zero layer of the reciprocal lattice to find the value of the correction appropriate to any reciprocal-lattice point. The necessary data for the construction of this chart are given in Table 5.2.5E.

5.2.5.2. EQUI-INCLINATION METHOD, $\mu = -\nu$ (Section 4.4.1(b))

Weissenberg cameras are often used in this position. The three equivalent expressions for L are

$$\left. \begin{aligned} L^{-1} &= \cos^2 \mu \sin Y \\ L^{-1} &= \sin 2\theta \frac{(\sin^2 \theta - \sin^2 \mu)^{\frac{1}{2}}}{\sin \theta} \\ \text{and } L^{-1} &= \xi \cos \theta \end{aligned} \right\} \quad \dots (19)$$

As before, $\cos^2 \mu$ is constant for each layer line. The Lorentz factor may therefore conveniently be found from the Buerger-Klein table of $\text{cosec } Y$.

Tunell [14] has evaluated (ξ, μ) curves of constant "rotation factor" $(\sin^2 \theta - \sin^2 \mu)^{\frac{1}{2}}/\sin \theta$. It is, however, much more convenient to be able to derive the value of Lp in one operation. Chia-Si Lu [13] has prepared a chart which covers the range $0 \leq \zeta \leq 1$, and for a given value of ζ gives $\cos^2 \mu \sin Y/(1 + \cos^2 2\theta)$ as a function of Y . Lu's chart can therefore be used in conjunction with the Weissenberg photograph to find the value of $(Lp)^{-1}$ for each reflection.

Kaan and Cole [11] have prepared a similar chart, but they have omitted the factor $\cos^2 \mu$, as it is constant on a given layer line. Their chart covers the range $0 \leq \mu \leq 30^\circ$. The necessary data for the construction of this chart are given in Table 5.2.5F.

Chia-Si Lu [13] and Cochran [5] have expressed $(Lp)^{-1}$ as a function of ξ and ζ . Curves on which the value of $\xi \cos \theta / (1 + \cos^2 2\theta)$ is constant are drawn on a chart which covers the whole range of values which ξ and ζ can assume. This chart is to be used in conjunction with a drawing of a zero layer of the reciprocal lattice. Data are given in Table 5.2.5G.

5.2.5.3. THE PRECESSION METHOD (C. E. Nordman)

The Lorentz factor for recording with the Buerger precession camera is extremely complicated. The camera is constructed so that the normal to the reciprocal-lattice layer being photographed moves on the surface of a circular cone of semi-angle $\bar{\mu}$. This precession takes place with a constant angular velocity Ω . In such circumstances ω is not constant, and L is found to depend on all three cylindrical polar co-ordinates $(\xi\zeta\tau)$ of a reciprocal-lattice point.† For the particular case $\bar{\mu}=30^\circ$ (a convenient value in practice) the functions $\{L(\xi 0 \tau)p\}^{-1}$ and $\{L(\xi \zeta \tau)p\}^{-1}$ have been evaluated and the results presented in the form of contoured charts by Waser [17], Burbank [4] and Grenville-Wells and Abrahams [10]. An extension of these calculations has been made, and the values of $(Lp)^{-1}$ corrections are presented in Table 5.2.5H, in the form of the radial co-ordinates of various contours of constant $(Lp)^{-1}$ where these intersect a set of "spokes" of given angular co-ordinates.

Table 5.2.5I (prepared by J. Kraut) gives relative values of $(Lp)^{-1}$ at points of a Cartesian co-ordinate system in the reciprocal plane, for zero-level precession photographs for *odd* precession angles between 11° and 29° . Values for *even* precession angles may be obtained by interpolation provided that points near to the outer edges of the tables are avoided. If preferred, the data can be normalized to a maximum Lp value of unity.

5.2.5.4. OTHER METHODS OF RECORDING

The Lorentz factor appropriate to the de Jong-Bouman method of recording has been derived by Bouman and de Jong [1] and by Buerger [2].

For the retigraph where there is no azimuthal variation, A. L. Mackay (*Acta Cryst.*, **13**, 240, 1960) gives the following previously unpublished formulae. For unpolarized incident radiation:

$$1/L^2 = \xi^2 \sin^2 \bar{\mu} - \frac{1}{4}(\zeta^2 - 2\zeta \cos \bar{\mu} + \xi^2)^2$$

$$\text{or } 1/L^2 = \xi^2 \cos^2 \mu - \frac{1}{4}(\zeta^2 - 2\zeta \sin \mu + \xi^2)^2$$

The angle $\bar{\mu}$ is defined in Section 5.2.5.3 and it is the complement of the angle μ as defined in Table 4.3.1 (p. 175) and again in Section 5.2.5.1. The expression is identical with the more usual form in terms of $\frac{1}{2}(1 + \cos^2 2\theta)$.

For monochromatized incident radiation:

$$p = \frac{1}{2} + \frac{1}{8} \cos^2 2\theta_M (2 - d^{*2})^2 + \frac{1}{8} d^{*4} (\cos^2 2\theta_M - 1) \tan^2 (\bar{\mu} + \mu')$$

where θ_M is the Bragg angle for the reflection from the monochromator; the axis about which the film plane is tilted lies in the plane of reflection of the mono-

chromator; μ' is the cone semi-angle for the layer in question; $d^* = \lambda/d$.

Kartha [12] has prepared a chart from which the value of $(Lp)^{-1}$ can be read off when the anti-equi-inclination method of recording zero-layer Weissenberg photographs has been used.

5.2.5.5. GENERAL REMARKS ON THE USE OF CHARTS AND TABLES

The methods which give Lp as the product of two factors, each of which must be looked up separately, are less convenient than the others. The methods of Buerger and Klein [3], Cox and Shaw [6], Tunell [14], and Goldschmidt and Pitt [9] fall in this category. The remaining methods may be divided into two groups:

- Those where Lp is expressed as a function of ζ (or μ) and Y . The charts are used in conjunction with the X-ray photograph.
- Those where Lp is expressed in terms of ξ and ζ . In this case the charts are used in conjunction with a drawing of a layer of the reciprocal lattice.

On a rotation photograph taken with a camera of radius r , the co-ordinates (xy) of a spot on the film are related to Y and ζ by the equations

$$x = rY, y = r\zeta/\sqrt{1 - \zeta^2}$$

(y is along the direction of the rotation axis). Table 5.2.5D gives the values of x , for a range of values of y , for which $(Lp)^{-1}$ assumes the values of 0, 0.1, 0.2, . . . , 2.0. The numbers refer to a camera of radius 5×2.865 cm, but the change to any other radius is a matter of simple proportion. The chart is symmetrical about the line $Y=90^\circ$.

From this table, charts appropriate to an n -level normal-beam Weissenberg photograph can also be constructed.

For an equi-inclination Weissenberg photograph, μ is constant and

$$(Lp)^{-1} = \frac{2 \cos^2 \mu \sin Y}{1 + \cos^2 2\theta} \quad \dots (20)$$

Table 5.2.5F gives the values of Y , for a number of values of μ , at which $2 \sin Y / (1 + \cos^2 2\theta)$ assumes the values 0, 0.1, 0.2, . . . , 2.0. From this table a chart can be constructed which is appropriate to an n -level equi-inclination Weissenberg photograph.

The remaining tables are for the construction of charts to be used with a drawing of the reciprocal lattice. Table 5.2.5E gives values of ξ , for a range of values of ζ , at which $(Lp)^{-1}$ assumes the values 0, 0.1, 0.2, . . . , 2.0. It is for the normal-beam method of recording. Table 5.2.5G contains the data for a similar chart appropriate to the equi-inclination method.

† Note that $(\xi\zeta\tau)$ as used here and by Waser, etc. [17] [4] [10], correspond to the $(\xi\zeta\phi)$ co-ordinates adopted in Section 4; ξ is the radial, ζ the axial and τ the angular cylindrical co-ordinate of the reciprocal lattice point $P(\xi\zeta\tau)$.

TABLE 5.2.5A

Lorentz-polarization Factor, $2L_p = \frac{1 + \cos^2 2\theta}{\sin 2\theta}$ as a Function of $\sin \theta$

$\sin \theta$	0.000	0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009
0.00	∞	1000	500.0	333.3	250.0	200.0	166.7	142.8	125.0	111.1
0.01	99.98	90.89	83.32	76.90	71.41	66.64	62.48	58.80	55.53	52.60
0.02	49.97	47.59	45.42	43.44	41.63	39.96	38.42	37.00	35.67	34.44
0.03	33.29	32.21	31.20	30.25	29.36	28.52	27.72	26.97	26.26	25.58
0.04	24.94	24.33	23.75	23.19	22.66	22.15	21.67	21.21	20.76	20.33
0.05	19.93	19.53	19.15	18.79	18.44	18.10	17.77	17.46	17.15	16.86
0.06	16.58	16.30	16.04	15.78	15.53	15.29	15.05	14.83	14.60	14.39
0.07	14.18	13.98	13.78	13.59	13.40	13.22	13.04	12.87	12.70	12.54
0.08	12.38	12.22	12.07	11.92	11.78	11.64	11.50	11.36	11.23	11.10
0.09	10.98	10.85	10.73	10.61	10.50	10.38	10.27	10.16	10.06	9.954
0.10	9.851	9.751	9.652	9.556	9.461	9.368	9.277	9.187	9.099	9.013
0.11	8.928	8.844	8.762	8.682	8.603	8.525	8.449	8.374	8.300	8.227
0.12	8.156	8.085	8.016	7.948	7.881	7.815	7.750	7.686	7.623	7.561
0.13	7.500	7.440	7.381	7.323	7.265	7.208	7.152	7.097	7.043	6.990
0.14	6.937	6.885	6.833	6.783	6.733	6.683	6.635	6.587	6.539	6.492
0.15	6.446	6.401	6.356	6.311	6.268	6.224	6.182	6.139	6.098	6.056
0.16	6.016	5.976	5.936	5.896	5.858	5.819	5.782	5.744	5.707	5.670
0.17	5.634	5.598	5.563	5.528	5.494	5.459	5.425	5.392	5.359	5.326
0.18	5.294	5.262	5.230	5.198	5.168	5.137	5.106	5.076	5.046	5.017
0.19	4.988	4.959	4.930	4.902	4.874	4.846	4.819	4.791	4.764	4.738
0.20	4.711	4.685	4.659	4.633	4.608	4.583	4.558	4.533	4.508	4.484
0.21	4.460	4.436	4.412	4.389	4.366	4.343	4.320	4.297	4.275	4.252
0.22	4.230	4.208	4.187	4.165	4.144	4.123	4.102	4.081	4.061	4.040
0.23	4.020	4.000	3.980	3.960	3.940	3.921	3.902	3.883	3.864	3.845
0.24	3.826	3.808	3.789	3.771	3.753	3.735	3.717	3.699	3.682	3.664
0.25	3.647	3.630	3.613	3.596	3.579	3.562	3.546	3.530	3.513	3.497
0.26	3.481	3.465	3.449	3.434	3.418	3.402	3.387	3.372	3.356	3.342
0.27	3.327	3.312	3.297	3.282	3.268	3.253	3.239	3.225	3.211	3.197
0.28	3.183	3.169	3.155	3.141	3.128	3.114	3.101	3.088	3.074	3.061
0.29	3.048	3.035	3.022	3.009	2.997	2.984	2.971	2.959	2.946	2.934
0.30	2.922	2.910	2.898	2.886	2.874	2.862	2.850	2.838	2.827	2.815
0.31	2.804	2.792	2.781	2.769	2.758	2.747	2.736	2.725	2.714	2.703
0.32	2.692	2.681	2.671	2.660	2.649	2.639	2.628	2.618	2.608	2.597
0.33	2.587	2.577	2.567	2.557	2.547	2.537	2.527	2.517	2.507	2.498
0.34	2.488	2.478	2.469	2.459	2.450	2.440	2.431	2.422	2.413	2.404
0.35	2.394	2.385	2.376	2.367	2.358	2.349	2.341	2.332	2.323	2.314
0.36	2.306	2.297	2.288	2.280	2.272	2.263	2.255	2.246	2.238	2.230
0.37	2.222	2.214	2.205	2.197	2.189	2.181	2.173	2.166	2.158	2.150
0.38	2.142	2.134	2.127	2.119	2.111	2.104	2.096	2.089	2.081	2.074
0.39	2.066	2.059	2.052	2.044	2.037	2.030	2.023	2.016	2.009	2.002
0.40	1.994	1.988	1.981	1.974	1.967	1.960	1.953	1.946	1.940	1.933
0.41	1.926	1.920	1.913	1.906	1.900	1.893	1.887	1.880	1.874	1.868
0.42	1.861	1.855	1.849	1.842	1.836	1.830	1.824	1.818	1.812	1.806
0.43	1.800	1.793	1.788	1.782	1.776	1.770	1.764	1.758	1.752	1.746
0.44	1.741	1.735	1.729	1.724	1.718	1.712	1.707	1.701	1.696	1.690
0.45	1.685	1.679	1.674	1.668	1.663	1.658	1.652	1.647	1.642	1.637
0.46	1.631	1.626	1.621	1.616	1.611	1.606	1.601	1.596	1.591	1.586
0.47	1.581	1.576	1.571	1.566	1.561	1.556	1.552	1.547	1.542	1.537
0.48	1.533	1.528	1.523	1.519	1.514	1.509	1.505	1.500	1.496	1.491
0.49	1.487	1.482	1.478	1.474	1.469	1.465	1.460	1.456	1.452	1.448

TABLE 5.2.5A (continued)

Lorentz-polarization Factor, $2Lp = \frac{1 + \cos^2 2\theta}{\sin 2\theta}$ as a Function of $\sin \theta$

$\sin \theta$	0.000	0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009
0.50	1.443	1.439	1.435	1.431	1.427	1.422	1.418	1.414	1.410	1.406
0.51	1.402	1.398	1.394	1.390	1.386	1.382	1.378	1.375	1.371	1.367
0.52	1.363	1.359	1.356	1.352	1.348	1.344	1.341	1.337	1.333	1.330
0.53	1.326	1.322	1.319	1.315	1.312	1.308	1.305	1.302	1.298	1.295
0.54	1.291	1.288	1.284	1.281	1.278	1.274	1.271	1.268	1.265	1.262
0.55	1.258	1.255	1.252	1.249	1.246	1.243	1.240	1.236	1.234	1.230
0.56	1.228	1.224	1.222	1.219	1.216	1.213	1.210	1.207	1.204	1.201
0.57	1.198	1.196	1.193	1.190	1.188	1.185	1.182	1.179	1.177	1.174
0.58	1.172	1.169	1.166	1.164	1.161	1.159	1.156	1.154	1.151	1.149
0.59	1.146	1.144	1.142	1.139	1.137	1.135	1.132	1.130	1.128	1.126
0.60	1.123	1.121	1.119	1.117	1.115	1.112	1.110	1.108	1.106	1.104
0.61	1.102	1.100	1.098	1.096	1.094	1.092	1.090	1.088	1.086	1.085
0.62	1.083	1.081	1.079	1.077	1.076	1.074	1.072	1.070	1.069	1.067
0.63	1.065	1.064	1.062	1.061	1.059	1.058	1.056	1.054	1.053	1.051
0.64	1.050	1.049	1.047	1.046	1.044	1.043	1.042	1.040	1.039	1.038
0.65	1.037	1.035	1.034	1.033	1.032	1.031	1.030	1.028	1.027	1.026
0.66	1.025	1.024	1.023	1.022	1.021	1.020	1.019	1.018	1.018	1.017
0.67	1.016	1.015	1.014	1.013	1.013	1.012	1.011	1.010	1.010	1.009
0.68	1.008	1.008	1.007	1.007	1.006	1.006	1.005	1.005	1.004	1.004
0.69	1.003	1.003	1.003	1.002	1.002	1.002	1.002	1.001	1.001	1.001
0.70	1.001	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
0.71	1.000	1.000	1.000	1.000	1.001	1.001	1.001	1.001	1.001	1.002
0.72	1.002	1.002	1.003	1.003	1.004	1.004	1.004	1.005	1.005	1.006
0.73	1.006	1.007	1.008	1.008	1.009	1.010	1.010	1.011	1.012	1.013
0.74	1.014	1.014	1.015	1.016	1.017	1.018	1.019	1.020	1.021	1.022
0.75	1.024	1.025	1.026	1.027	1.028	1.030	1.031	1.032	1.034	1.035
0.76	1.037	1.038	1.040	1.041	1.043	1.044	1.046	1.048	1.049	1.051
0.77	1.053	1.055	1.056	1.058	1.060	1.062	1.064	1.066	1.068	1.070
0.78	1.072	1.075	1.077	1.079	1.081	1.084	1.086	1.088	1.091	1.093
0.79	1.096	1.098	1.101	1.104	1.106	1.109	1.112	1.115	1.118	1.120
0.80	1.123	1.126	1.129	1.132	1.136	1.139	1.142	1.145	1.148	1.152
0.81	1.155	1.159	1.162	1.166	1.169	1.173	1.177	1.180	1.184	1.188
0.82	1.192	1.196	1.200	1.204	1.208	1.212	1.217	1.221	1.225	1.230
0.83	1.234	1.239	1.243	1.248	1.253	1.258	1.262	1.267	1.272	1.277
0.84	1.282	1.288	1.293	1.298	1.304	1.309	1.315	1.320	1.326	1.332
0.85	1.338	1.344	1.350	1.356	1.362	1.368	1.375	1.381	1.388	1.394
0.86	1.401	1.408	1.415	1.422	1.429	1.436	1.443	1.451	1.458	1.466
0.87	1.473	1.481	1.489	1.497	1.505	1.513	1.522	1.530	1.539	1.548
0.88	1.556	1.566	1.575	1.584	1.593	1.603	1.612	1.622	1.632	1.642
0.89	1.653	1.663	1.674	1.684	1.695	1.706	1.718	1.729	1.741	1.752
0.90	1.764	1.777	1.789	1.802	1.814	1.827	1.841	1.854	1.868	1.882
0.91	1.896	1.910	1.925	1.940	1.955	1.970	1.986	2.002	2.019	2.035
0.92	2.052	2.070	2.087	2.105	2.124	2.142	2.161	2.181	2.201	2.221
0.93	2.242	2.263	2.284	2.307	2.329	2.352	2.376	2.400	2.425	2.451
0.94	2.477	2.503	2.531	2.559	2.588	2.617	2.648	2.679	2.711	2.744
0.95	2.778	2.813	2.849	2.886	2.924	2.964	3.004	3.047	3.090	3.136
0.96	3.182	3.231	3.282	3.334	3.388	3.445	3.504	3.566	3.630	3.698
0.97	3.769	3.843	3.921	4.004	4.090	4.182	4.280	4.383	4.493	4.611
0.98	4.737	4.873	5.020	5.179	5.353	5.543	5.753	5.986	6.247	6.542
0.99	6.880	7.272	7.733	8.289	8.978	9.861	11.05	12.80	15.71	22.26

TABLE 5.2.5B
Correcting Factor $\frac{4Lp}{\sin \theta} = \frac{1 + \cos^2 2\theta}{\sin^2 \theta \cos \theta}$ as a Function of $\sin \theta$

$\sin \theta$	0.000	0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009
0.02	4997	4532	4129	3778	3469	3197	2956	2740	2548	2375
0.03	2219	2078	1950	1834	1727	1630	1540	1458	1382	1312
0.04	1247	1187	1131	1079	1030	984.7	942.2	902.4	865.1	830.0
0.05	797.0	765.9	736.7	709.0	682.9	658.2	634.8	612.6	591.5	571.6
0.06	552.6	534.5	517.3	500.9	485.3	470.4	456.1	442.5	429.5	417.1
0.07	405.2	393.8	382.8	372.3	362.2	352.6	343.3	334.3	325.7	317.5
0.08	309.5	301.8	294.5	287.3	280.5	273.8	267.4	261.3	255.3	249.5
0.09	243.9	238.5	233.3	228.3	223.4	218.6	214.0	209.6	205.3	201.1
0.10	197.0	193.1	189.3	185.5	181.9	178.4	175.0	171.7	168.5	165.4
0.11	162.3	159.4	156.5	153.7	150.9	148.3	145.7	143.1	140.7	138.3
0.12	135.9	133.6	131.4	129.2	127.1	125.0	123.0	121.0	119.1	117.2
0.13	115.4	113.6	111.8	110.1	108.4	106.8	105.2	103.6	102.1	100.6
0.14	99.10	97.65	96.24	94.86	93.51	92.18	90.89	89.61	88.37	87.15
0.15	85.95	84.78	83.63	82.50	81.40	80.31	79.25	78.21	77.18	76.18
0.16	75.20	74.23	73.28	72.35	71.44	70.54	69.66	68.79	67.94	67.11
0.17	66.28	65.48	64.69	63.91	63.14	62.39	61.65	60.92	60.21	59.51
0.18	58.82	58.14	57.47	56.81	56.17	55.53	54.91	54.29	53.69	53.09
0.19	52.50	51.92	51.36	50.80	50.25	49.70	49.17	48.64	48.12	47.61
0.20	47.11	46.62	46.13	45.65	45.18	44.71	44.25	43.80	43.35	42.91
0.21	42.48	42.05	41.63	41.21	40.80	40.40	40.00	39.60	39.22	38.84
0.22	38.46	38.09	37.72	37.36	37.00	36.65	36.30	35.96	35.62	35.29
0.23	34.96	34.63	34.31	33.99	33.68	33.37	33.07	32.77	32.47	32.17
0.24	31.88	31.60	31.32	31.04	30.76	30.49	30.22	29.95	29.69	29.43
0.25	29.18	28.92	28.67	28.43	28.18	27.94	27.70	27.47	27.23	27.00
0.26	26.78	26.55	26.33	26.11	25.89	25.68	25.47	25.26	25.05	24.84
0.27	24.64	24.44	24.24	24.05	23.85	23.66	23.47	23.28	23.10	22.91
0.28	22.73	22.55	22.38	22.20	22.03	21.85	21.68	21.52	21.35	21.18
0.29	21.02	20.86	20.70	20.54	20.38	20.23	20.08	19.93	19.78	19.63
0.30	19.48	19.33	19.19	19.05	18.91	18.77	18.63	18.49	18.35	18.22
0.31	18.09	17.96	17.82	17.70	17.57	17.44	17.32	17.19	17.07	16.95
0.32	16.83	16.71	16.59	16.47	16.35	16.24	16.12	16.01	15.90	15.79
0.33	15.68	15.57	15.46	15.36	15.25	15.15	15.04	14.94	14.84	14.74
0.34	14.64	14.54	14.44	14.34	14.24	14.15	14.05	13.96	13.87	13.77
0.35	13.68	13.59	13.50	13.41	13.32	13.24	13.15	13.06	12.98	12.89
0.36	12.81	12.73	12.64	12.56	12.48	12.40	12.32	12.24	12.16	12.09
0.37	12.01	11.93	11.86	11.78	11.71	11.63	11.56	11.49	11.42	11.34
0.38	11.27	11.20	11.13	11.06	11.00	10.93	10.86	10.79	10.73	10.66
0.39	10.60	10.53	10.47	10.40	10.34	10.28	10.22	10.15	10.09	10.03
0.40	9.973	9.913	9.854	9.795	9.736	9.679	9.621	9.564	9.508	9.452
0.41	9.396	9.341	9.286	9.232	9.178	9.124	9.071	9.019	8.966	8.915
0.42	8.863	8.812	8.761	8.711	8.661	8.612	8.562	8.514	8.465	8.417
0.43	8.370	8.322	8.275	8.229	8.182	8.136	8.091	8.046	8.001	7.956
0.44	7.912	7.868	7.825	7.781	7.738	7.696	7.654	7.612	7.570	7.529
0.45	7.488	7.447	7.406	7.366	7.326	7.287	7.248	7.208	7.170	7.131
0.46	7.093	7.055	7.018	6.980	6.943	6.907	6.870	6.834	6.798	6.762
0.47	6.727	6.692	6.657	6.622	6.588	6.553	6.519	6.486	6.452	6.419
0.48	6.386	6.353	6.321	6.288	6.256	6.224	6.193	6.162	6.130	6.100
0.49	6.069	6.038	6.008	5.978	5.948	5.918	5.889	5.860	5.831	5.802

TABLE 5.2.5B (continued)

Correcting Factor $\frac{4Lp}{\sin \theta} = \frac{1 + \cos^2 2\theta}{\sin^2 \theta \cos \theta}$ as a Function of $\sin \theta$

$\sin \theta$	0.000	0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009
0.50	5.774	5.745	5.717	5.689	5.661	5.634	5.606	5.579	5.552	5.525
0.51	5.499	5.472	5.446	5.420	5.394	5.368	5.343	5.318	5.292	5.267
0.52	5.243	5.218	5.194	5.169	5.145	5.121	5.098	5.074	5.051	5.027
0.53	5.004	4.981	4.959	4.936	4.914	4.891	4.869	4.847	4.826	4.804
0.54	4.782	4.761	4.740	4.719	4.698	4.677	4.657	4.636	4.616	4.596
0.55	4.576	4.556	4.536	4.517	4.497	4.478	4.459	4.440	4.421	4.402
0.56	4.384	4.365	4.347	4.329	4.311	4.293	4.275	4.258	4.240	4.223
0.57	4.205	4.188	4.171	4.154	4.138	4.121	4.105	4.088	4.072	4.056
0.58	4.040	4.024	4.008	3.993	3.977	3.962	3.946	3.931	3.916	3.901
0.59	3.886	3.872	3.857	3.843	3.828	3.814	3.800	3.786	3.772	3.758
0.60	3.744	3.731	3.717	3.704	3.691	3.678	3.665	3.652	3.639	3.626
0.61	3.614	3.601	3.588	3.576	3.564	3.552	3.540	3.528	3.516	3.504
0.62	3.493	3.481	3.470	3.459	3.448	3.436	3.425	3.414	3.404	3.393
0.63	3.382	3.372	3.361	3.351	3.341	3.331	3.320	3.311	3.301	3.291
0.64	3.281	3.272	3.262	3.253	3.243	3.234	3.225	3.216	3.207	3.198
0.65	3.189	3.181	3.172	3.164	3.155	3.147	3.139	3.130	3.122	3.114
0.66	3.106	3.099	3.091	3.083	3.076	3.068	3.061	3.054	3.046	3.039
0.67	3.032	3.025	3.018	3.012	3.005	2.998	2.992	2.985	2.979	2.972
0.68	2.966	2.960	2.954	2.948	2.942	2.936	2.931	2.925	2.919	2.914
0.69	2.908	2.903	2.898	2.893	2.888	2.883	2.878	2.873	2.868	2.864
0.70	2.859	2.854	2.850	2.846	2.841	2.837	2.833	2.829	2.825	2.821
0.71	2.817	2.814	2.810	2.806	2.803	2.799	2.796	2.793	2.790	2.786
0.72	2.783	2.780	2.778	2.775	2.772	2.770	2.767	2.764	2.762	2.760
0.73	2.758	2.755	2.753	2.751	2.749	2.748	2.746	2.744	2.743	2.741
0.74	2.740	2.738	2.737	2.736	2.735	2.734	2.733	2.732	2.731	2.730
0.75	2.730	2.729	2.729	2.728	2.728	2.728	2.728	2.728	2.728	2.728
0.76	2.728	2.728	2.729	2.729	2.730	2.730	2.731	2.732	2.733	2.734
0.77	2.735	2.736	2.737	2.738	2.740	2.741	2.743	2.744	2.746	2.748
0.78	2.750	2.752	2.754	2.756	2.759	2.761	2.764	2.766	2.769	2.772
0.79	2.774	2.777	2.780	2.784	2.787	2.790	2.794	2.797	2.801	2.804
0.80	2.808	2.812	2.816	2.820	2.825	2.829	2.834	2.838	2.843	2.848
0.81	2.852	2.857	2.862	2.868	2.873	2.878	2.884	2.890	2.895	2.901
0.82	2.907	2.913	2.920	2.926	2.932	2.939	2.946	2.953	2.960	2.967
0.83	2.974	2.981	2.989	2.996	3.004	3.012	3.020	3.028	3.037	3.045
0.84	3.054	3.062	3.071	3.080	3.089	3.099	3.108	3.118	3.128	3.138
0.85	3.148	3.158	3.168	3.179	3.190	3.201	3.212	3.223	3.235	3.246
0.86	3.258	3.270	3.282	3.295	3.307	3.320	3.333	3.346	3.360	3.373
0.87	3.387	3.401	3.415	3.430	3.444	3.459	3.474	3.490	3.506	3.521
0.88	3.538	3.554	3.570	3.588	3.605	3.622	3.640	3.658	3.676	3.695
0.89	3.714	3.733	3.752	3.772	3.792	3.813	3.834	3.855	3.877	3.899
0.90	3.921	3.944	3.967	3.990	4.014	4.038	4.063	4.088	4.114	4.140
0.91	4.167	4.194	4.221	4.249	4.278	4.307	4.337	4.367	4.398	4.429
0.92	4.461	4.494	4.528	4.562	4.596	4.632	4.668	4.705	4.743	4.781
0.93	4.821	4.861	4.902	4.945	4.988	5.032	5.077	5.124	5.171	5.220
0.94	5.270	5.321	5.373	5.427	5.482	5.539	5.597	5.657	5.719	5.782
0.95	5.848	5.915	5.985	6.056	6.130	6.207	6.286	6.367	6.452	6.539
0.96	6.630	6.724	6.822	6.924	7.030	7.140	7.255	7.375	7.501	7.633
0.97	7.771	7.916	8.068	8.229	8.399	8.579	8.770	8.972	9.188	9.420
0.98	9.668	9.935	10.22	10.54	10.88	11.25	11.67	12.13	12.65	13.23
0.99	13.90	14.68	15.59	16.70	18.06	19.82	22.20	25.67	31.49	44.57

TABLE 5.2.5C
Correcting Factor $\frac{4Lp}{\cos \theta} = \frac{1 + \cos^2 2\theta}{\sin \theta \cos^2 \theta}$ as a Function of $\sin \theta$

$\sin \theta$	0.000	0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009
0.00	∞	2000	1000	666.7	500.0	400.0	333.3	285.7	250.0	222.2
0.01	200.0	181.8	166.6	153.8	142.8	133.3	125.0	117.6	111.1	105.2
0.02	100.0	95.20	90.86	86.91	83.29	80.00	76.87	74.02	71.37	68.91
0.03	66.61	64.45	62.44	60.54	58.76	57.07	55.48	53.98	52.56	51.20
0.04	49.92	48.70	47.54	46.43	45.37	44.35	43.39	42.46	41.57	40.72
0.05	39.90	39.11	38.36	37.63	36.93	35.25	35.60	34.97	34.37	33.78
0.06	33.21	32.67	32.13	31.62	31.12	30.64	30.17	29.72	29.28	28.85
0.07	28.43	28.03	27.63	27.25	26.88	26.52	26.16	25.82	25.49	25.16
0.08	24.84	24.53	24.23	23.93	23.64	23.36	23.09	22.82	22.55	22.30
0.09	22.04	21.80	21.56	21.32	21.09	20.86	20.64	20.43	20.21	20.01
0.10	19.80	19.60	19.41	19.21	19.02	18.84	18.66	18.48	18.31	18.13
0.11	17.96	17.80	17.64	17.48	17.32	17.16	17.01	16.86	16.72	16.57
0.12	16.43	16.29	16.15	16.02	15.88	15.75	15.63	15.50	15.37	15.25
0.13	15.13	15.01	14.89	14.78	14.66	14.55	14.44	14.33	14.22	14.12
0.14	14.01	13.91	13.81	13.71	13.61	13.51	13.41	13.32	13.22	13.13
0.15	13.04	12.95	12.86	12.77	12.69	12.60	12.52	12.43	12.35	12.27
0.16	12.19	12.11	12.03	11.95	11.88	11.80	11.73	11.65	11.58	11.51
0.17	11.43	11.36	11.29	11.23	11.16	11.09	11.02	10.96	10.89	10.83
0.18	10.76	10.70	10.64	10.58	10.51	10.45	10.39	10.33	10.28	10.22
0.19	10.16	10.10	10.05	9.992	9.936	9.882	9.828	9.774	9.721	9.669
0.20	9.617	9.565	9.514	9.464	9.414	9.364	9.315	9.266	9.218	9.170
0.21	9.123	9.076	9.030	8.984	8.938	8.893	8.848	8.804	8.760	8.716
0.22	8.673	8.630	8.588	8.546	8.504	8.463	8.422	8.381	8.341	8.301
0.23	8.261	8.222	8.183	8.144	8.106	8.068	8.030	7.993	7.956	7.919
0.24	7.883	7.846	7.811	7.775	7.740	7.705	7.670	7.635	7.601	7.567
0.25	7.533	7.500	7.467	7.434	7.401	7.369	7.336	7.304	7.273	7.241
0.26	7.210	7.179	7.148	7.118	7.087	7.057	7.027	6.998	6.968	6.939
0.27	6.910	6.881	6.852	6.824	6.796	6.768	6.740	6.712	6.685	6.658
0.28	6.630	6.604	6.577	6.550	6.524	6.498	6.472	6.446	6.420	6.395
0.29	6.370	6.345	6.320	6.295	6.270	6.246	6.222	6.198	6.174	6.150
0.30	6.126	6.102	6.079	6.056	6.033	6.010	5.987	5.965	5.942	5.920
0.31	5.898	5.876	5.854	5.832	5.810	5.789	5.767	5.746	5.725	5.704
0.32	5.683	5.662	5.642	5.621	5.601	5.581	5.560	5.540	5.521	5.501
0.33	5.481	5.462	5.442	5.423	5.404	5.385	5.366	5.347	5.328	5.310
0.34	5.291	5.273	5.255	5.236	5.218	5.200	5.182	5.165	5.147	5.130
0.35	5.112	5.095	5.077	5.060	5.043	5.026	5.009	4.992	4.976	4.959
0.36	4.943	4.926	4.910	4.894	4.878	4.862	4.846	4.830	4.814	4.798
0.37	4.783	4.767	4.752	4.736	4.721	4.706	4.691	4.676	4.661	4.646
0.38	4.631	4.617	4.602	4.588	4.573	4.559	4.544	4.530	4.516	4.502
0.39	4.488	4.474	4.460	4.447	4.433	4.419	4.406	4.392	4.379	4.366
0.40	4.352	4.339	4.326	4.313	4.300	4.287	4.274	4.262	4.249	4.236
0.41	4.224	4.211	4.199	4.186	4.174	4.162	4.150	4.138	4.126	4.114
0.42	4.102	4.090	4.078	4.066	4.055	4.043	4.032	4.020	4.009	3.998
0.43	3.986	3.975	3.964	3.953	3.942	3.931	3.920	3.909	3.898	3.887
0.44	3.877	3.866	3.856	3.845	3.835	3.824	3.814	3.804	3.793	3.783
0.45	3.773	3.763	3.753	3.743	3.733	3.723	3.713	3.704	3.694	3.684
0.46	3.675	3.665	3.656	3.646	3.637	3.628	3.618	3.609	3.600	3.591
0.47	3.582	3.573	3.564	3.555	3.546	3.537	3.529	3.520	3.511	3.503
0.48	3.494	3.486	3.477	3.469	3.460	3.452	3.444	3.436	3.427	3.419
0.49	3.411	3.403	3.395	3.387	3.380	3.372	3.364	3.356	3.348	3.341

TABLE 5.2.5C (continued)

Correcting Factor $\frac{4Lp}{\cos \theta} = \frac{1 + \cos^2 2\theta}{\sin \theta \cos^2 \theta}$ as a Function of $\sin \theta$

$\sin \theta$	0.000	0.001	0.002	0.003	0.004	0.005	0.006	0.007	0.008	0.009
0.50	3.333	3.326	3.318	3.311	3.304	3.296	3.289	3.282	3.274	3.267
0.51	3.260	3.253	3.246	3.239	3.232	3.225	3.218	3.212	3.205	3.198
0.52	3.192	3.185	3.178	3.172	3.166	3.159	3.153	3.146	3.140	3.134
0.53	3.128	3.122	3.115	3.109	3.103	3.097	3.092	3.086	3.080	3.074
0.54	3.068	3.063	3.057	3.051	3.046	3.040	3.035	3.029	3.024	3.019
0.55	3.013	3.008	3.003	2.998	2.993	2.988	2.983	2.978	2.973	2.968
0.56	2.963	2.958	2.954	2.949	2.944	2.940	2.935	2.931	2.926	2.922
0.57	2.917	2.913	2.909	2.905	2.900	2.896	2.892	2.888	2.884	2.880
0.58	2.876	2.872	2.869	2.865	2.861	2.858	2.854	2.850	2.847	2.843
0.59	2.840	2.837	2.833	2.830	2.827	2.824	2.820	2.817	2.814	2.811
0.60	2.808	2.805	2.803	2.800	2.797	2.794	2.792	2.789	2.787	2.784
0.61	2.782	2.779	2.777	2.775	2.772	2.770	2.768	2.766	2.764	2.762
0.62	2.760	2.758	2.756	2.755	2.753	2.751	2.750	2.748	2.747	2.745
0.63	2.744	2.742	2.741	2.740	2.739	2.738	2.737	2.736	2.735	2.734
0.64	2.733	2.732	2.732	2.731	2.730	2.730	2.729	2.729	2.728	2.728
0.65	2.728	2.728	2.728	2.728	2.728	2.728	2.728	2.728	2.728	2.729
0.66	2.729	2.730	2.730	2.731	2.731	2.732	2.733	2.734	2.734	2.736
0.67	2.737	2.738	2.739	2.740	2.742	2.743	2.744	2.746	2.748	2.749
0.68	2.751	2.753	2.755	2.757	2.759	2.761	2.763	2.765	2.768	2.770
0.69	2.773	2.775	2.778	2.781	2.784	2.786	2.789	2.792	2.796	2.799
0.70	2.802	2.806	2.809	2.813	2.816	2.820	2.824	2.828	2.832	2.836
0.71	2.840	2.845	2.849	2.854	2.858	2.863	2.868	2.872	2.878	2.883
0.72	2.888	2.893	2.898	2.904	2.910	2.915	2.921	2.927	2.933	2.939
0.73	2.945	2.952	2.958	2.965	2.972	2.978	2.985	2.992	2.999	3.007
0.74	3.014	3.022	3.029	3.037	3.045	3.053	3.061	3.070	3.078	3.086
0.75	3.095	3.104	3.113	3.122	3.131	3.141	3.150	3.160	3.170	3.180
0.76	3.190	3.200	3.211	3.221	3.232	3.243	3.254	3.266	3.277	3.288
0.77	3.300	3.312	3.324	3.337	3.349	3.362	3.374	3.388	3.401	3.414
0.78	3.428	3.442	3.456	3.470	3.484	3.499	3.514	3.528	3.544	3.559
0.79	3.575	3.591	3.607	3.623	3.640	3.657	3.674	3.691	3.708	3.726
0.80	3.744	3.763	3.781	3.800	3.819	3.839	3.858	3.878	3.898	3.919
0.81	3.940	3.961	3.982	4.004	4.026	4.048	4.071	4.094	4.117	4.141
0.82	4.165	4.189	4.214	4.239	4.265	4.290	4.317	4.343	4.370	4.398
0.83	4.426	4.454	4.482	4.511	4.541	4.571	4.601	4.632	4.663	4.695
0.84	4.727	4.760	4.793	4.827	4.862	4.896	4.932	4.968	5.004	5.041
0.85	5.079	5.117	5.156	5.196	5.236	5.276	5.318	5.360	5.403	5.446
0.86	5.491	5.538	5.581	5.628	5.675	5.723	5.772	5.822	5.872	5.924
0.87	5.976	6.030	6.084	6.139	6.195	6.252	6.310	6.370	6.430	6.491
0.88	6.554	6.618	6.683	6.749	6.816	6.885	6.955	7.026	7.099	7.173
0.89	7.249	7.326	7.405	7.485	7.567	7.650	7.736	7.823	7.912	8.003
0.90	8.096	8.190	8.287	8.386	8.488	8.591	8.697	8.805	8.916	9.029
0.91	9.145	9.264	9.385	9.510	9.637	9.768	9.902	10.04	10.18	10.32
0.92	10.47	10.62	10.78	10.94	11.11	11.28	11.45	11.63	11.81	12.00
0.93	12.20	12.40	12.61	12.82	13.04	13.27	13.50	13.74	13.99	14.25
0.94	14.52	14.79	15.08	15.38	15.68	16.00	16.33	16.68	17.03	17.41
0.95	17.79	18.19	18.61	19.05	19.51	19.98	20.48	21.00	21.55	22.13
0.96	22.73	23.37	24.03	24.74	25.48	26.27	27.11	27.99	28.93	29.93
0.97	31.00	32.15	33.37	34.69	36.11	37.64	39.30	41.11	43.08	45.23
0.98	47.61	50.23	53.15	56.41	60.08	64.24	68.99	74.48	80.88	88.44
0.99	97.52	108.6	122.5	140.3	164.1	197.4	247.3	330.5	496.7	994.1

TABLE 5.2.5D

Data for the Construction of Constant $(Lp)^{-1}$ Curves for Rotation and Oscillation Photographs

The table gives the relationship between the x and y film co-ordinates in cm for constant $(Lp)^{-1}$ values from $Y=0^\circ$ to 45° or 90° to 45° . Data for camera radius of 5×2.865 cm; y is parallel to the rotation axis.

$\begin{matrix} y \\ (Lp)^{-1} \end{matrix}$	0.0	1.5	2.0	2.5	5.0	7.5	10.0	12.5	15.0	17.5	20.0	22.5	25.0
0.10	1.43	1.43	1.43	1.43	1.43	1.44	1.46	1.49	1.53	1.58	1.65	1.72	1.80
0.20	2.83	2.83	2.83	2.83	2.84	2.86	2.89	2.96	3.04	3.15	3.28	3.43	3.59
0.30	4.18	4.18	4.18	4.18	4.20	4.23	4.29	4.39	4.53	4.70	4.90	5.12	5.37
0.40	5.46	5.47	5.47	5.47	5.49	5.55	5.64	5.78	5.97	6.21	6.49	6.80	7.15
0.50	6.68	6.68	6.68	6.69	6.73	6.80	6.94	7.13	7.38	7.69	8.06	8.48	8.95
0.60	7.82	7.83	7.83	7.84	7.89	8.00	8.17	8.42	8.75	9.15	9.62	10.16	10.77
0.70	8.89	8.90	8.91	8.91	8.99	9.13	9.36	9.67	10.08	10.59	11.19	11.88	12.68
0.80	9.90	9.91	9.92	9.93	10.03	10.22	10.50	10.89	11.40	12.03	12.79	13.68	14.75
0.90	10.86	10.87	10.88	10.90	11.02	11.25	11.60	12.09	12.71	13.50	14.47	15.68	17.26
1.00	11.77	11.78	11.80	11.82	11.97	12.26	12.68	13.27	14.05	15.05	16.35	18.18	
1.10	12.64	12.66	12.68	12.70	12.89	13.23	13.75	14.47	15.45	16.77	18.75		
1.20	13.48	13.51	13.53	13.55	13.79	14.20	14.83	15.72	17.00	18.97			
1.30	14.30	14.34	14.36	14.39	14.67	15.17	15.94	17.09	18.91				
1.40	15.12	15.16	15.19	15.22	15.60	16.17	17.13	18.71					
1.50	15.94	15.98	16.02	16.06	16.47	17.22	18.50	21.56					
1.60	16.77	16.83	16.87	16.93	17.43	18.41	20.42						
1.70	17.66	17.73	17.78	17.86	18.50	19.91							
1.80	18.64	18.73	18.80	18.90	19.82								
1.90	19.83	19.97	20.08	20.24									
1.95	20.63	20.84	21.02	21.30									
1.98	21.33	21.71	22.27										

These figures give the
x film co-ordinates in cm.

TABLE 5.2.5E

Values of ξ , for a Range of Values of ζ , at which $(Lp)^{-1}$ assumes the Values 0, 0.1, 0.2, . . . , 2.0

$$\text{For normal-beam recording } (Lp)^{-1} = \frac{2(\sin^2 2\theta - \zeta^2)^{\frac{1}{2}}}{1 + \cos^2 2\theta}$$

$(Lp)^{-1} \backslash \zeta$	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8
0	0	0.005	0.020	0.046	0.083	0.134	0.200	0.286	0.400
0.1	0.100	0.100	0.101	0.108	0.127	0.164	0.220	0.299	0.409
0.2	0.197	0.197	0.196	0.198	0.207	0.229	0.270	0.336	0.436
0.3	0.291	0.290	0.287	0.288	0.292	0.306	0.335	0.388	0.477
0.4	0.379	0.378	0.376	0.375	0.376	0.384	0.405	0.448	0.526
0.5	0.462	0.461	0.458	0.456	0.455	0.460	0.476	0.512	0.582
0.6	0.539	0.538	0.536	0.532	0.530	0.533	0.545	0.576	0.641
0.7	0.611	0.610	0.607	0.603	0.601	0.602	0.613	0.641	0.703
0.8	0.678	0.677	0.674	0.670	0.667	0.668	0.677	0.704	0.767
0.9	0.740	0.739	0.736	0.733	0.730	0.730	0.740	0.767	0.834
1.0	0.798	0.798	0.795	0.792	0.789	0.790	0.800	0.830	0.906
1.1	0.854	0.853	0.851	0.848	0.846	0.848	0.860	0.894	0.991
1.2	0.907	0.906	0.904	0.902	0.901	0.905	0.920	0.962	
1.3	0.958	0.957	0.955	0.954	0.955	0.961	0.981	1.038	
1.4	1.007	1.007	1.006	1.006	1.008	1.018	1.046	1.144	
1.5	1.056	1.056	1.056	1.057	1.063	1.078	1.122		
1.6	1.105	1.105	1.107	1.110	1.120	1.146	1.281		
1.7	1.156	1.157	1.160	1.167	1.185	1.240			
1.8	1.211	1.213	1.219	1.234	1.275				
1.9	1.276	1.280	1.294	1.344					
2.0	1.414								
1.9	1.540	1.530	1.498	1.419					
1.8	1.591	1.584	1.560	1.516	1.433				
1.7	1.632	1.625	1.605	1.568	1.508	1.401			
1.6	1.667	1.661	1.642	1.609	1.557	1.479	1.281		
1.5	1.698	1.693	1.675	1.644	1.597	1.529	1.421		
1.4	1.728	1.722	1.705	1.676	1.632	1.570	1.478	1.308	
1.3	1.756	1.751	1.734	1.706	1.664	1.605	1.522	1.394	
1.2	1.783	1.777	1.761	1.734	1.694	1.638	1.560	1.448	
1.1	1.809	1.804	1.788	1.761	1.722	1.668	1.594	1.490	1.318
1.0	1.834	1.829	1.813	1.787	1.749	1.696	1.625	1.527	1.378
0.9	1.858	1.853	1.838	1.812	1.774	1.722	1.653	1.559	1.423
0.8	1.882	1.877	1.862	1.836	1.799	1.748	1.680	1.589	1.460
0.7	1.904	1.900	1.885	1.859	1.822	1.771	1.704	1.615	1.492
0.6	1.926	1.921	1.906	1.881	1.844	1.793	1.727	1.639	1.519
0.5	1.946	1.941	1.926	1.901	1.864	1.813	1.747	1.661	1.543
0.4	1.964	1.959	1.944	1.918	1.881	1.831	1.765	1.679	1.563
0.3	1.979	1.974	1.959	1.933	1.896	1.846	1.780	1.694	1.579
0.2	1.990	1.985	1.970	1.944	1.907	1.857	1.791	1.705	1.590
0.1	1.998	1.993	1.977	1.952	1.914	1.864	1.798	1.712	1.598
0	2.000	1.995	1.980	1.954	1.917	1.866	1.800	1.714	1.600

TABLE 5.2.5F

Data for the Construction of Constant $(Lp)^{-1}$ Curves for Equi-inclination Weissenberg PhotographsThe table gives the relationship between Y and μ in degrees for constant $(Lp)^{-1}$ values

$(Lp)^{-1} \backslash \mu$	0.0	2.5	5.0	7.5	10.0	12.5	15.0	17.5	20.0	22.5	25.0	27.5	30.0
0.10	5.7	5.7	5.6	5.5	5.4	5.2	5.0	4.8	4.5	4.3	4.0	3.8	3.6
0.20	11.3	11.3	11.1	10.9	10.7	10.3	9.9	9.5	9.0	8.5	8.1	7.6	7.1
0.30	16.7	16.7	16.5	16.2	15.8	15.3	14.8	14.1	13.4	12.7	12.0	11.3	10.7
0.40	21.9	21.8	21.6	21.2	20.7	20.1	19.4	18.6	17.7	16.9	15.9	15.1	14.2
0.50	26.7	26.6	26.4	26.0	25.4	24.7	23.9	22.9	21.9	20.9	19.8	18.7	17.7
0.60	31.3	31.2	30.9	30.5	29.8	29.0	28.1	27.1	25.9	24.7	23.5	22.3	21.1
0.70	35.6	35.5	35.2	34.7	34.0	33.2	32.2	31.1	29.8	28.5	27.2	25.8	24.5
0.80	39.6	39.5	39.2	38.7	38.0	37.1	36.1	34.9	33.6	32.2	30.7	29.3	27.9
0.90	43.4	43.3	43.0	42.5	41.8	40.9	39.8	38.6	37.2	35.8	34.2	32.7	31.3
1.00	47.1	47.0	46.6	46.1	45.4	44.5	43.4	42.1	40.7	39.2	37.7	36.1	34.6
1.10	50.5	50.4	50.1	49.6	48.9	47.9	46.8	45.6	44.2	42.6	41.1	39.5	37.9
1.20	53.9	53.8	53.5	53.0	52.2	51.3	50.2	49.0	47.5	46.0	44.4	42.8	41.2
1.30	57.2	57.1	56.8	56.3	55.6	54.6	53.5	52.3	50.9	49.4	47.8	46.2	44.6
1.40	60.5	60.4	60.1	59.5	58.8	57.9	56.9	55.6	54.2	52.7	51.2	49.6	48.1
1.50	63.7	63.6	63.3	62.8	62.1	61.3	60.2	59.0	57.7	56.2	54.7	53.1	51.4
1.60	67.1	67.0	66.7	66.2	65.5	64.7	63.7	62.5	61.2	59.8	58.3	56.9	55.5
1.70	70.6	70.5	70.3	69.8	69.1	68.3	67.3	66.2	65.0	63.6	62.3	61.0	59.8
1.80	74.6	74.5	74.2	73.7	73.1	72.3	71.4	70.4	69.2	68.0	66.8	65.7	64.7
1.90	79.3	79.2	79.0	78.6	78.0	77.3	76.4	75.5	74.5	73.5	72.6	72.0	71.9
1.95	82.5	82.4	82.2	81.8	81.3	80.6	79.8	79.0	78.2	77.5	77.2	77.7	
1.98	85.3	85.2	85.0	84.6	84.1	83.5	82.9	82.3	81.9	82.3			
2.00	90.0												
1.98	94.7	94.6	94.4	94.1	93.6	92.8	91.9	90.6	88.9	86.1			
1.95	97.5	97.4	97.2	96.8	96.4	95.8	95.0	93.9	92.6	90.9	88.6	85.3	
1.90	100.7	100.6	100.4	100.1	99.7	99.1	98.4	97.5	96.4	95.0	93.3	91.1	88.4
1.80	105.4	105.4	105.2	105.0	104.6	104.1	103.4	102.7	101.7	100.6	99.3	97.7	95.7
1.70	109.4	109.3	109.2	108.9	108.6	108.1	107.6	106.9	106.1	105.1	103.9	102.6	101.0
1.60	112.9	112.9	112.7	112.5	112.2	111.8	111.3	110.7	110.0	109.1	108.1	106.9	105.6
1.50	116.3	116.2	116.1	115.9	115.6	115.3	114.8	114.3	113.6	112.9	112.0	111.0	109.8
1.40	119.5	119.5	119.4	119.2	119.0	118.6	118.2	117.8	117.2	116.5	115.7	114.9	113.9
1.30	122.8	122.8	122.7	122.5	122.3	122.0	121.6	121.2	120.7	120.1	119.5	118.7	117.8
1.20	126.1	126.1	126.0	125.8	125.6	125.4	125.1	124.7	124.3	123.8	123.2	122.5	121.8
1.10	129.5	129.4	129.4	129.2	129.1	128.9	128.6	128.3	127.9	127.5	127.0	126.4	125.8
1.00	132.9	132.9	132.9	132.8	132.6	132.4	132.2	131.9	131.6	131.3	130.9	130.4	129.9
0.90	136.6	136.6	136.5	136.4	136.3	136.2	136.0	135.8	135.5	135.2	134.9	134.5	134.1
0.80	140.4	140.4	140.3	140.3	140.2	140.1	139.9	139.7	139.5	139.3	139.1	138.8	138.4
0.70	144.4	144.4	144.4	144.3	144.3	144.2	144.1	143.9	143.8	143.6	143.4	143.2	143.0
0.60	148.7	148.7	148.7	148.7	148.6	148.5	148.5	148.4	148.3	148.1	148.0	147.9	147.7
0.50	153.3	153.3	153.3	153.2	153.2	153.2	153.1	153.1	153.0	152.9	152.8	152.7	152.6
0.40	158.1	158.1	158.1	158.1	158.1	158.1	158.0	158.0	158.0	157.9	157.9	157.8	157.8
0.30	163.3	163.3	163.3	163.3	163.3	163.3	163.2	163.2	163.2	163.2	163.2	163.1	163.1
0.20	168.7	168.7	168.7	168.7	168.7	168.7	168.7	168.7	168.7	168.7	168.6	168.6	168.6
0.10	174.3	174.3	174.3	174.3	174.3	174.3	174.3	174.3	174.3	174.3	174.3	174.3	174.3

Points of inflection for $(Lp)^{-1}=1.95$, $\mu=43.2^\circ$ and $Y=80.5^\circ$; for $(Lp)^{-1}=1.98$, $\mu=34.4^\circ$ and $Y=84.5^\circ$.

It should be noted that in this table the function designated $(Lp)^{-1}$ is $2 \sin Y/(1 + \cos^2 2\theta)$. The true value of $(Lp)^{-1}$ is in fact $2 \cos^2 \mu \sin Y/(1 + \cos^2 2\theta)$, but the factor $\cos^2 \mu$ has been omitted, as it is constant for all reflections on the same layer line.

TABLE 5.2.5G

Values of ξ , for a Range of Values of ζ , at which $(L_p)^{-1}$ assumes the Values 0, 0.1, 0.2, . . . , 2.0

$$\text{For equi-inclination recording } (L_p)^{-1} = \frac{2\xi \cos \theta}{1 + \cos^2 2\theta}.$$

$\zeta \backslash (L_p)^{-1}$	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0	1.2	1.4	1.6
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0.1	0.100	0.099	0.098	0.096	0.094	0.091	0.087	0.084	0.080	0.076	0.072	0.067	0.070	0.090
0.2	0.197	0.196	0.194	0.191	0.186	0.180	0.173	0.166	0.158	0.151	0.144	0.135	0.141	0.184
0.3	0.291	0.290	0.287	0.282	0.275	0.267	0.257	0.246	0.235	0.224	0.214	0.202	0.212	0.284
0.4	0.379	0.378	0.374	0.368	0.360	0.349	0.337	0.324	0.310	0.296	0.284	0.269	0.286	0.399
0.5	0.462	0.461	0.456	0.449	0.439	0.427	0.413	0.398	0.382	0.366	0.351	0.336	0.363	0.562
0.6	0.539	0.538	0.533	0.525	0.514	0.501	0.486	0.468	0.451	0.433	0.418	0.403	0.445	
0.7	0.611	0.609	0.604	0.596	0.584	0.570	0.554	0.536	0.517	0.499	0.483	0.471	0.537	
0.8	0.678	0.676	0.671	0.662	0.650	0.635	0.618	0.600	0.581	0.562	0.547	0.541	0.654	
0.9	0.740	0.738	0.733	0.724	0.712	0.697	0.680	0.661	0.642	0.624	0.610	0.614		
1.0	0.798	0.797	0.791	0.783	0.771	0.756	0.739	0.720	0.702	0.685	0.673	0.695		
1.1	0.854	0.852	0.847	0.838	0.826	0.812	0.795	0.778	0.760	0.746	0.738	0.792		
1.2	0.907	0.905	0.900	0.891	0.880	0.866	0.850	0.834	0.819	0.808	0.807			
1.3	0.958	0.956	0.951	0.943	0.932	0.919	0.905	0.890	0.878	0.873	0.883			
1.4	1.007	1.005	1.001	0.993	0.983	0.972	0.959	0.947	0.940	0.944	0.981			
1.5	1.056	1.055	1.050	1.044	1.035	1.025	1.015	1.008	1.009	1.034				
1.6	1.105	1.104	1.100	1.095	1.088	1.080	1.075	1.076	1.096					
1.7	1.156	1.155	1.152	1.148	1.144	1.141	1.144	1.166						
1.8	1.211	1.211	1.209	1.208	1.209	1.216	1.252							
1.9	1.276	1.277	1.279	1.286	1.307									
2.0	1.414													
1.9	1.540	1.534	1.516	1.483	1.424									
1.8	1.591	1.587	1.572	1.547	1.509	1.454	1.360							
1.7	1.632	1.628	1.615	1.593	1.560	1.515	1.454	1.364						
1.6	1.667	1.663	1.651	1.630	1.601	1.561	1.509	1.439	1.340					
1.5	1.698	1.695	1.683	1.664	1.637	1.600	1.552	1.491	1.412	1.299				
1.4	1.728	1.724	1.714	1.695	1.669	1.635	1.590	1.534	1.464	1.373	1.238			
1.3	1.756	1.752	1.742	1.725	1.700	1.667	1.625	1.573	1.508	1.427	1.321			
1.2	1.783	1.779	1.769	1.753	1.729	1.697	1.657	1.608	1.547	1.473	1.380			
1.1	1.809	1.805	1.796	1.780	1.756	1.726	1.688	1.641	1.583	1.514	1.429	1.167		
1.0	1.834	1.831	1.821	1.806	1.783	1.754	1.717	1.672	1.618	1.552	1.473	1.248		
0.9	1.858	1.855	1.846	1.831	1.809	1.781	1.745	1.702	1.651	1.588	1.513	1.311		
0.8	1.882	1.879	1.870	1.855	1.834	1.807	1.773	1.731	1.680	1.621	1.551	1.365	1.041	
0.7	1.904	1.902	1.893	1.879	1.858	1.832	1.799	1.758	1.710	1.653	1.586	1.413	1.142	
0.6	1.926	1.923	1.915	1.901	1.881	1.855	1.823	1.784	1.738	1.683	1.619	1.456	1.216	
0.5	1.946	1.943	1.935	1.921	1.902	1.877	1.846	1.808	1.763	1.711	1.650	1.495	1.277	0.873
0.4	1.964	1.961	1.953	1.940	1.921	1.897	1.866	1.830	1.786	1.736	1.677	1.530	1.328	1.013
0.3	1.979	1.976	1.968	1.955	1.937	1.913	1.883	1.848	1.806	1.756	1.700	1.559	1.370	1.097
0.2	1.990	1.988	1.980	1.967	1.949	1.926	1.897	1.862	1.820	1.772	1.717	1.581	1.402	1.154
0.1	1.998	1.995	1.987	1.975	1.957	1.934	1.905	1.870	1.830	1.783	1.728	1.595	1.421	1.188
0	2.000	1.997	1.990	1.977	1.960	1.936	1.908	1.873	1.833	1.786	1.732	1.600	1.428	1.200

TABLE 5.2.5H

(C. E. NORDMAN)

Lorentz-polarization Corrections for the Precession Method, $\bar{\mu} \approx 30^\circ$

A. Zero Level

Entries are the values of the radial co-ordinate $10^3 \times \xi$ (in dimensionless reciprocal-lattice units) for which $(Lp)^{-1}$ has the value given in column at left,

while values of the angular co-ordinate τ are given at the top of each column. Values and locations of maxima are given at the bottom of each column. The horizontal direction on the film corresponds to $\tau=0^\circ$.

$(Lp)^{-1} \backslash \tau$	0°	10°	20°	30°	40°	50°	60°	70°	80°	90°
0.05	30	30	31	32	33	35	36	38	38	38
0.10	59	60	62	63	67	71	72	76	77	78
0.15	89	90	92	94	100	106	108	115	117	118
0.20	118	120	123	126	134	141	146	153	156	158
0.25	149	151	154	158	168	176	182	190	193	195
0.30	179	181	186	191	202	212	219	228	232	233
0.35	210	212	218	224	236	247	254	265	269	271
0.40	241	243	250	257	270	281	290	301	306	307
0.45	274	276	282	290	304	317	326	337	343	345
0.50	306	308	314	323	338	350	361	372	378	380
0.55	338	340	347	356	372	386	396	407	413	415
0.60	370	373	380	390	406	421	431	443	449	451
0.65	404	407	415	425	442	457	467	478	484	485
0.70	442	445	454	464	480	495	505	515	521	522
0.75	482	485	493	504	519	532	542	552	556	559
0.80	524	528	536	547	561	571	580	588	593	595
0.85	573	575	583	594	605	613	621	627	630	632
0.90	630	633	639	646	653	660	665	668	670	672
0.925	671	674	678	681	685	688	691	693	694	695
0.95				761	734	725	724	723	722	721
0.975							765	756	751	749
1.000										817
0.975							826	851	864	870
0.95				764	807	835	860	873	883	886
0.925	799	803	811	826	842	861	879	890	897	900
0.90	826	829	836	849	862	878	893	901	907	910
0.85	865	866	872	882	892	903	914	921	925	927
0.80	889	891	896	904	912	920	929	935	938	939
0.75	909	910	914	921	927	934	941	946	948	949
0.70	924	926	929	934	939	946	951	954	957	958
0.60	949	950	952	956	959	963	967	969	970	971
0.50	966	967	968	971	973	975	978	979	980	980
0.25	992									995
0.00	1000									1000
$(Lp)^{-1}$ at max.	0.941	0.942	0.945	0.951	0.958	0.969	0.982	0.991	0.997	1.000
Corresponding value of $10^3 \cdot \xi$	741	745	751	762	773	786	798	808	814	817

TABLE 5.2.5H (continued)

Lorentz-polarization Corrections for the Precession Method, $\bar{\mu}=30^\circ$

B. Upper Levels

Entries are the values of the radial co-ordinate $10^3 \times \xi$ for which $(Lp)^{-1}$ has the value given in the column at left, while the axial co-ordinate ζ and the angular co-ordinate τ have the values given at the top of each table. Values and locations of maxima for each ζ and τ are given at the bottom of the tables. The ξ values were derived from a set of graphs of $(Lp)^{-1}$ vs. ξ for ζ and $\tau = \text{const.}$ by means of graphical interpolation. No attempt has been made to eliminate possible interpolation errors by smoothing in the

directions of the ζ and τ co-ordinates. The scale of $(Lp)^{-1}$ is the same as that used in the zero-level table. The horizontal direction on the film corresponds to $\tau=0$.

ξ and ζ are in dimensionless reciprocal-lattice units. There are two columns under each ζ ; $10^3 \times \xi$ increases downward in the first column until the maximum $(Lp)^{-1}$ is reached, and then increases upward in the second column as $(Lp)^{-1}$ decreases. All values are not included in the second column, since the increments are so small.

$\tau=0^\circ$

<div><div><div><div></div><div>ζ</div><div>$(Lp)^{-1}$</div></div></div></div>	0.01		0.05		0.10		0.15		0.20		0.25		0.35	
0.0	17	1017	78	1078	143	1143	198	1198	246	1246	288	1288	357	1357
0.1	62		101		155		208		253		294		360	
0.2	120		140		184		230		272		308		370	
0.3	178	1005	187	1070	220		258		296		328		386	
0.4	238	997	236	1062	258		288		322		352		404	
0.5	299	985	287	1054	299		322		350		376		424	
0.6	365	969	339	1043	341		356		380		402		445	
0.7	434	948	396	1029	386		395		412		430		468	
0.8	503	917	454	1011	434		434		446		459		490	
0.9	595	872	519	987	484	1078	475		480		490		514	
1.0			589	954	536	1059	519		516		520		538	
1.1			680	895	593	1036	563		555		552		563	
1.2					657	1004	612	1100	594		587		589	
1.3					740	954	664	1075	636		621		616	
1.4							725	1043	682		659		645	
1.5							800	992	730	1106	697		674	
1.6									786	1073	741	1158	705	
1.7									859	1023	788	1132	738	
1.8											842	1098	772	1228
1.9											923	1035	808	1209
2.0													846	1188
2.1													895	1156
2.2													954	1108
(Lp) ⁻¹ at max.	0.987		1.159		1.364		1.558		1.744		1.923		2.256	
Corresponding value of 10 ³ . ξ	752		800		854		904		945		981		1038	

5.2. INTENSITY OF RADIATION DIFFRACTED BY A CRYSTAL

TABLE 5.2.5H (*continued*)Lorentz-polarization Corrections for the Precession Method, $\bar{\mu}=30^\circ$ $\tau=15^\circ$

ζ (Lp) ⁻¹	0.01		0.05		0.10		0.15		0.20		0.25		0.35	
0.0	17	1017	78	1078	143	1143	198	1198	246	1246	288	1288	357	1357
0.1	63		101		156		208		253		293		360	
0.2	120		142		186		231		271		308		370	
0.3	180	1005	189	1069	222		260		296		328		385	
0.4	243	997	239	1062	260		291		324		351		404	
0.5	306	986	290	1055	302		325		351		378		424	
0.6	371	970	343	1044	344		360		383		405		446	
0.7	440	950	402	1031	391		400		416		433		470	
0.8	512	919	462	1013	439		440		450		463		493	
0.9	606	874	531	990	490	1080	482		486		495		517	
1.0			600	956	543	1062	526		522		526		542	
1.1			695	898	601	1038	572		562		558		568	
1.2					671	1005	623	1102	602		593		595	
1.3					753	952	678	1077	645		629		623	
1.4							738	1042	692		667		652	
1.5							818	988	740	1107	708		682	
1.6									802	1074	753	1157	714	
1.7									886	1013	802	1133	745	
1.8											857	1096	780	1230
1.9											961	1014	818	1210
2.0													860	1187
2.1													909	1154
2.2													980	1100
(Lp) ⁻¹ at max. Corresponding value of 10 ³ . ξ	0.984		1.153		1.353		1.544		1.730		1.906		2.231	
	760		805		860		910		952		988		1042	

5.2. INTENSITY OF RADIATION DIFFRACTED BY A CRYSTAL

TABLE 5.2.5H (*continued*)Lorentz-polarization Corrections for the Precession Method, $\bar{\mu}=30^\circ$ $\tau=30^\circ$

ζ (Lp) ⁻¹	0.01		0.05		0.10		0.15		0.20		0.25		0.35	
0.0	17	1017	78	1078	143	1143	198	1198	246	1246	288	1288	357	1357
0.1	66		102		156		208		252		292		360	
0.2	127		144		185		230		270		308		370	
0.3	191	1006	196	1070	225		260		294		328		385	
0.4	255	1000	248	1064	268		295		324		353		404	
0.5	320	990	304	1058	312		331		356		381		425	
0.6	388	976	359	1048	358		370		390		410		448	
0.7	458	956	421	1035	406		412		426		440		474	
0.8	539	929	486	1020	460		455		462		473		499	
0.9	633	884	551	997	512	1087	499		500		506		526	
1.0			627	965	569	1069	546		540		540		552	
1.1			729	904	631	1045	598		582		576		581	
1.2					702	1012	650	1108	626		614		610	
1.3					799	953	708	1084	671		652		640	
1.4							770	1050	719		694		672	
1.5							876	976	775	1113	738		704	
1.6									841	1077	787	1166	738	
1.7											839	1136	774	
1.8											906	1093	812	1235
1.9													852	1214
2.0													899	1188
2.1													960	1146
(Lp) ⁻¹ at max. Corresponding value of 10 ³ . ξ	0.978		1.144		1.334		1.518		1.699		1.867		2.179	
	774		821		878		928		971		1014		1060	

5.2. INTENSITY OF RADIATION DIFFRACTED BY A CRYSTAL

TABLE 5.2.5H (continued)

Lorentz-polarization Corrections for the Precession Method, $\bar{\mu}=30^\circ$ $\tau=45^\circ$

ζ (Lp) ⁻¹	0.01		0.05		0.10		0.15		0.20		0.25		0.35	
0.0	17	1017	78	1078	143	1143	198	1198	246	1246	288	1288	357	1357
0.1	70		102		154		206		252		292		360	
0.2	136		149		186		229		269		306		368	
0.3	202	1008	206	1070	231		262		296		326		383	
0.4	270	1001	264	1066	278		301		329		354		402	
0.5	339	993	323	1060	327		342		364		385		427	
0.6	410	980	386	1052	378		386		402		418		452	
0.7	484	965	447	1040	433		433		442		453		480	
0.8	564	941	515	1026	488		480		484		490		510	
0.9	650	904	582	1006	546	1093	529		527		527		540	
1.0			659	980	604	1078	582		570		566		570	
1.1			756	926	669	1058	634		616		606		603	
1.2					740	1025	690	1121	663		647		635	
1.3					836	973	746	1097	711		690		670	
1.4							814	1064	763		734		705	
1.5							926	995	821	1128	781		740	
1.6									887	1090	830	1177	779	
1.7											887	1150	818	
1.8											962	1100	856	1246
1.9													903	1225
2.0													954	1195
2.1													1025	1146
(Lp) ⁻¹ at max. Corresponding value of $10^3 \cdot \xi$	0.985		1.144		1.330		1.506		1.679		1.841		2.134	
	800		851		908		960		1000		1040		1091	

5.2. INTENSITY OF RADIATION DIFFRACTED BY A CRYSTAL

TABLE 5.2.5H (*continued*)Lorentz-polarization Corrections for the Precession Method, $\bar{\mu}=30^\circ$ $\tau=60^\circ$

ζ (Lp) ⁻¹	0.01		0.05		0.10		0.15		0.20		0.25		0.35	
0.0	17	1017	78	1078	143	1143	198	1198	246	1246	288	1288	357	1357
0.1	74		101		154		204		251		291		360	
0.2	145		155		186		228		267		304		367	
0.3	218	1009	218		236		262		294		324		380	
0.4	290	1002	282		290		308		330		354		400	
0.5	362	995	345	1062	346		355		372		388		426	
0.6	432	985	410	1055	404		408		417		426		454	
0.7	504	971	476	1046	462		460		462		468		487	
0.8	580	952	542	1034	520		512		510		510		521	
0.9	661	922	608	1017	579		563		558		552		557	
1.0	780	849	680	994	637	1087	616		605		598		592	
1.1			763	956	698	1070	670		654		642		629	
1.2					763	1044	723		702		685		667	
1.3					847	1002	779	1110	750		730		706	
1.4							842	1085	800		775		743	
1.5							927	1030	853	1141	821		781	
1.6									916	1110	868	1190	820	
1.7											921	1166	860	
1.8											991	1127	901	1258
													946	1238
2.0													996	1212
2.1													1067	1164
(Lp) ⁻¹ at max. Corresponding value of 10 ³ . ξ	1.008		1.167		1.351		1.522		1.688		1.848		2.130	
	818		870		930		985		1026		1064		1115	

5.2. INTENSITY OF RADIATION DIFFRACTED BY A CRYSTAL

TABLE 5.2.5H (continued)

Lorentz-polarization Corrections for the Precession Method, $\bar{\mu}=30^\circ$ $\tau=75^\circ$

ζ (Lp) ⁻¹	0.01		0.05		0.10		0.15		0.20		0.25		0.35	
0.0	17	1017	78	1078	143	1143	198	1198	246	1246	288	1288	357	1357
0.1	78		100		152		204		250		291		359	
0.2	154		160		186		226		265		303		366	
0.3	228	1009	228		240		262		292		322		379	
0.4	302	1004	300		300		312		332		352		398	
0.5	375	998	363	1063	362		367		378		390		424	
0.6	446	988	430	1058	424		424		429		434		456	
0.7	515	975	496	1050	485		480		482		482		492	
0.8	587	958	558	1038	543		534		532		528		532	
0.9	661	932	621	1024	600		589		583		575		572	
1.0	753	886	689	1004	656	1093	641		632		622		612	
1.1			762	974	714	1078	692		679		667		653	
1.2					772	1055	743		725		712		694	
1.3					845	1020	794	1122	772		756		734	
1.4							852	1097	819		798		773	
1.5							921	1059	868	1154	843		810	
1.6									922	1125	889	1200	848	
1.7									1005	1076	936	1179	886	
1.8											993	1149	927	1268
1.9													968	1250
2.0													1013	1225
2.1													1073	1190
(Lp) ⁻¹ at max. Corresponding value of $10^3 \cdot \xi$	1.032		1.189		1.377		1.550		1.716		1.873		2.146	
	829		880		951		1002		1042		1077		1132	

5.2. INTENSITY OF RADIATION DIFFRACTED BY A CRYSTAL

TABLE 5.2.5H (*continued*)Lorentz-polarization Corrections for the Precession Method, $\bar{\mu}=30^\circ$ $\tau=90^\circ$

ζ (Lp) ⁻¹	0.01		0.05		0.10		0.15		0.20		0.25		0.35	
0.0	17	1017	78	1078	143	1143	198	1198	246	1246	288	1288	357	1357
0.1	80		100		152		204		251		291		359	
0.2	157		162		186		224		266		303		366	
0.3	232	1008	234		240		261		292		322		378	
0.4	307	1004	302		307		313		333		352		398	
0.5	380	998	372	1064	369		371		380		391		422	
0.6	448	989	436	1058	433		432		433		438		456	
0.7	517	978	502	1050	494		489		487		488		494	
0.8	586	961	563	1040	550		545		540		537		535	
0.9	656	937	625	1026	608		598		592		586		578	
1.0	744	893	690	1008	663	1095	650		641		632		620	
1.1			758	979	717	1080	700		688		678		663	
1.2			866	890	773	1060	749		734		722		705	
1.3					842	1030	798	1124	779		765		744	
1.4							852	1103	826		808		782	
1.5							918	1071	872	1160	850		820	
1.6									924	1132	893	1205	858	
1.7									993	1094	939	1184	896	
1.8											992	1156	934	1275
1.9													974	1256
2.0													1016	1232
2.1													1070	1199
(Lp) ⁻¹ at max. Corresponding value of $10^3 \cdot \xi$	1.043		1.202		1.387		1.562		1.728		1.886		2.158	
	832		885		955		1008		1048		1082		1140	

TABLE 5.2.5I

(J. KRAUT)

 $(Lp)^{-1}$ for Zero-level Precession Photographs, for Odd Values of $\bar{\mu}$

The following tables list Lorentz-polarization correction factors $(Lp)^{-1}$ for zero-level precession photographs only, and are designed to facilitate the convenient preparation of charts such as that published by Waser [17] for the precession angle 30° . They represent Waser's function, suitably scaled, evaluated at points 0.05 reciprocal-lattice units (r.l.u.) apart in one quadrant of the zero-level reciprocal lattice plane. The remaining quadrants are obtained by reflection across

the axes. The horizontal table co-ordinate corresponds to the horizontal direction on the film.

Tables are given for odd precession angles $\bar{\mu}$ between 11° and 29° ; values for even precession angles may be obtained by interpolation, provided that points near the outer edges of the tables are avoided.

The tables were prepared with the aid of an IBM-650 digital computer.

The reciprocal-lattice units are dimensionless.

 $\bar{\mu}=11^\circ$

r.l.u.	0.00	0.05	0.10	0.15	0.20	0.25	0.30	0.35	
									$\rightarrow \tau=0^\circ$
0.00	—	0650	1268	1817	2254	2513	2484	1883	
0.05	0627	0896	1396	1892	2295	2525	2463	1799	
0.10	1228	1371	1706	2085	2398	2545	2380	1483	
0.15	1771	1856	2069	2319	2508	2521	2163	0342	
0.20	2217	2264	2381	2504	2541	2354	1612		
0.25	2500	2516	2544	2528	2362	1822			
0.30	2506	2487	2407	2190	1630				
0.35	1932	1845	1522	0351					
	\downarrow								$\tau=90^\circ$

 $\bar{\mu}=13^\circ$

r.l.u.	0.00	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40
0.00	—	0553	1086	1580	2011	2346	2540	2519	2116
0.05	0525	0758	1196	1649	2054	2371	2548	2506	2071
0.10	1037	1164	1469	1830	2171	2435	2561	2459	1915
0.15	1518	1598	1806	2072	2328	2513	2556	2343	1565
0.20	1949	2000	2137	2315	2478	2563	2484	2085	0575
0.25	2300	2330	2409	2503	2563	2519	2260	1488	
0.30	2526	2537	2560	2565	2499	2271	1673		
0.35	2546	2536	2492	2379	2119	1509			
0.40	2181	2135	1976	1615	0593				

5.2. INTENSITY OF RADIATION DIFFRACTED BY A CRYSTAL

TABLE 5.2.5I (*continued*) $(Lp)^{-1}$ for Zero-level Precession Photographs, for Odd Values of $\bar{\mu}$ $\bar{\mu}=15^\circ$

r.l.u.	0.00	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40	0.45	0.50	$\rightarrow \tau=0^\circ$
0.00	—	0481	0950	1395	1800	2147	2415	2567	2550	2256	1327	
0.05	0449	0656	1045	1455	1841	2175	2430	2572	2542	2229	1239	
0.10	0891	1006	1282	1619	1955	2251	2473	2581	2512	2136	0905	
0.15	1316	1391	1587	1846	2118	2359	2529	2582	2443	1946		
0.20	1714	1765	1904	2096	2299	2474	2576	2549	2298	1568		
0.25	2070	2104	2199	2331	2465	2563	2577	2438	2005	0565		
0.30	2360	2382	2439	2513	2574	2582	2480	2168	1357			
0.35	2552	2560	2580	2592	2568	2459	2182	1527				
0.40	2585	2579	2554	2489	2346	2046	1380					
0.45	2338	2310	2216	2020	1629	0586						
0.50	1410	1316	0961									
$\downarrow \tau=90^\circ$												

 $\bar{\mu}=17^\circ$

r.l.u.	0.00	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40	0.45	0.50	0.55
0.00	—	0426	0845	1247	1623	1963	2251	2471	2594	2581	2354	1716
0.05	0390	0576	0926	1300	1660	1989	2270	2481	2597	2575	2336	1669
0.10	0776	0881	1134	1446	1766	2065	2321	2511	2604	2555	2275	1514
0.15	1154	1223	1406	1653	1922	2179	2398	2552	2607	2510	2156	1178
0.20	1516	1565	1700	1891	2106	2313	2485	2591	2591	2420	1939	
0.25	1854	1890	1989	2133	2295	2449	2565	2608	2531	2249	1533	
0.30	2158	2183	2253	2354	2465	2560	2609	2572	2386	1921	0415	
0.35	2409	2425	2469	2528	2585	2614	2581	2433	2077	1208		
0.40	2579	2586	2603	2619	2614	2561	2414	2093	1374			
0.45	2624	2620	2606	2567	2481	2308	1969	1232				
0.50	2453	2435	2375	2253	2028	1602	0433					
0.55	1838	1789	1622	1263								

5.2. INTENSITY OF RADIATION DIFFRACTED BY A CRYSTAL

TABLE 5.2.5I (*continued*) $(Lp)^{-1}$ for Zero-level Precession Photographs, for Odd Values of $\bar{\mu}$ $\bar{\mu}=19^\circ$

r.l.u.	0.00	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40	0.45	0.50	0.55	0.60	0.65	$\rightarrow \tau=0^\circ$
0.00	—	0383	0761	1127	1476	1800	2090	2335	2520	2623	2612	2429	1948	0325	
0.05	0343	0512	0831	1174	1509	1825	2109	2348	2528	2625	2608	2416	1918		
0.10	0684	0780	1013	1303	1605	1896	2161	2385	2549	2630	2593	2374	1822		
0.15	1020	1084	1256	1490	1748	2006	2243	2441	2580	2633	2562	2293	1633		
0.20	1348	1395	1524	1710	1924	2143	2344	2508	2611	2625	2502	2152	1280		
0.25	1663	1699	1798	1944	2115	2292	2452	2574	2632	2591	2393	1910	0331		
0.30	1960	1986	2061	2173	2305	2438	2552	2624	2623	2507	2196	1468			
0.35	2228	2247	2301	2382	2474	2562	2624	2634	2557	2332	1832				
0.40	2452	2465	2500	2550	2602	2639	2638	2569	2383	1984	1024				
0.45	2610	2616	2631	2648	2654	2630	2548	2367	2002	1196					
0.50	2665	2663	2654	2631	2578	2470	2267	1886	1048						
0.55	2548	2536	2495	2414	2269	2015	1546								
0.60	2106	2074	1971	1768	1386	0358									
0.65	0363														
\downarrow	$\tau=90^\circ$														

 $\bar{\mu}=21^\circ$

r.l.u.	0.00	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40	0.45	0.50	0.55	0.60	0.65	0.70
0.00	—	0348	0692	1029	1353	1660	1943	2196	2408	2566	2654	2644	2491	2107	1173
0.05	0304	0460	0754	1070	1383	1682	1960	2209	2417	2572	2655	2640	2482	2086	1113
0.10	0607	0697	0913	1183	1468	1747	2011	2246	2443	2587	2659	2629	2451	2020	0905
0.15	0908	0968	1130	1351	1598	1850	2090	2306	2485	2610	2661	2607	2392	1895	0274
0.20	1205	1250	1373	1552	1761	1980	2192	2383	2537	2636	2657	2564	2293	1681	
0.25	1496	1530	1627	1771	1945	2130	2310	2469	2591	2656	2637	2490	2132	1303	
0.30	1777	1804	1880	1995	2136	2286	2432	2555	2639	2660	2585	2360	1865	0279	
0.35	2044	2064	2123	2213	2322	2438	2546	2628	2665	2628	2478	2137	1375		
0.40	2286	2301	2345	2411	2490	2570	2636	2670	2647	2535	2274	1729			
0.45	2493	2503	2532	2575	2622	2662	2679	2652	2552	2329	1882	0765			
0.50	2644	2649	2663	2680	2692	2684	2640	2532	2316	1903	0965				
0.55	2709	2708	2704	2690	2656	2587	2455	2220	1789	0785					
0.60	2633	2624	2595	2538	2438	2270	1984	1460							
0.65	2302	2280	2209	2074	1841	1427	0305								
0.70	1328	1261	1025	0310											

5.2. INTENSITY OF RADIATION DIFFRACTED BY A CRYSTAL

TABLE 5.2.5I (continued)

(Lp)⁻¹ for Zero-level Precession Photographs, for Odd Values of $\bar{\mu}$ $\bar{\mu}=23^\circ$

r.l.u.	0.00	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40	0.45	0.50	0.55	0.60	0.65	0.70	0.75	$\rightarrow \tau=0^\circ$
0.00	—	0319	0636	0947	1249	1539	1812	2063	2286	2472	2611	2686	2677	2546	2226	1528	
0.05	0271	0417	0689	0983	1275	1559	1828	2076	2296	2479	2615	2687	2674	2538	2210	1492	
0.10	0542	0626	0830	1082	1350	1618	1874	2112	2323	2499	2626	2690	2665	2514	2161	1378	
0.15	0812	0870	1022	1232	1468	1711	1948	2171	2368	2530	2644	2692	2648	2470	2071	1149	
0.20	1082	1125	1243	1414	1617	1832	2046	2248	2427	2570	2664	2689	2616	2397	1924	0664	
0.25	1349	1382	1476	1617	1788	1975	2163	2340	2495	2615	2682	2676	2563	2282	1686		
0.30	1613	1639	1714	1829	1972	2130	2291	2441	2568	2657	2691	2643	2472	2100	1272		
0.35	1869	1890	1950	2044	2161	2291	2422	2541	2635	2688	2678	2574	2322	1801			
0.40	2113	2130	2178	2252	2345	2446	2546	2631	2686	2693	2626	2445	2068	1245			
0.45	2338	2351	2387	2443	2512	2584	2650	2695	2703	2652	2507	2209	1607				
0.50	2534	2543	2567	2605	2648	2688	2715	2712	2660	2529	2268	1764	0205				
0.55	2682	2687	2700	2716	2731	2734	2712	2646	2510	2257	1787	0596					
0.60	2757	2757	2755	2747	2726	2680	2592	2436	2164	1671	0211						
0.65	2713	2706	2685	2644	2573	2454	2259	1935	1332								
0.70	2460	2443	2392	2295	2134	1870	1409										
0.75	1756	1716	1585	1322	0763												
\downarrow $\tau=90^\circ$																	

 $\bar{\mu}=25^\circ$

r.l.u.	0.00	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40	0.45	0.50	0.55	0.60	0.65	0.70	0.75	0.80
0.00	—	0295	0589	0878	1161	1435	1696	1942	2167	2367	2532	2655	2720	2710	2594	2318	1755
0.05	0243	0380	0635	0909	1183	1452	1710	1953	2176	2374	2537	2658	2721	2708	2588	2306	1730
0.10	0486	0566	0758	0996	1249	1504	1752	1987	2203	2394	2552	2666	2722	2700	2569	2269	1652
0.15	0730	0785	0930	1129	1354	1588	1820	2042	2247	2428	2576	2679	2723	2686	2534	2200	1505
0.20	0975	1016	1129	1293	1489	1698	1911	2116	2306	2473	2607	2695	2721	2662	2478	2091	1252
0.25	1220	1252	1342	1479	1647	1831	2021	2207	2379	2527	2642	2710	2712	2621	2391	1923	0757
0.30	1464	1490	1564	1678	1820	1980	2147	2310	2460	2587	2679	2720	2689	2555	2259	1656	
0.35	1707	1728	1789	1883	2003	2139	2282	2421	2546	2647	2710	2716	2643	2448	2053	1189	
0.40	1945	1962	2011	2089	2189	2302	2420	2532	2630	2699	2726	2688	2556	2275	1714		
0.45	2174	2187	2227	2290	2370	2460	2552	2635	2700	2732	2713	2617	2403	1985	1057		
0.50	2387	2398	2429	2477	2537	2603	2667	2717	2743	2728	2649	2472	2132	1450			
0.55	2576	2584	2605	2638	2678	2717	2749	2760	2737	2660	2498	2195	1617				
0.60	2724	2729	2740	2757	2773	2782	2773	2735	2647	2481	2186	1641					
0.65	2809	2809	2809	2806	2793	2762	2701	2593	2407	2092	1516						
0.70	2790	2786	2770	2739	2686	2599	2459	2234	1861	1141							
0.75	2595	2583	2543	2470	2351	2164	1863	1335									
0.80	2050	2022	1931	1761	1464	0885											

5.2. INTENSITY OF RADIATION DIFFRACTED BY A CRYSTAL

TABLE 5.2.5I (continued)

(Lp)⁻¹ for Zero-level Precession Photographs, for Odd Values of $\bar{\mu}$ $\bar{\mu}=27^\circ$

r.l.u.	0.00	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40	0.45	0.50	0.55	0.60	0.65	0.70	0.75	0.80	0.85	0.90
0.00	—	0275	0549	0819	1085	1344	1594	1833	2056	2260	2440	2589	2698	2756	2744	2638	2393	1915	0772
0.05	0219	0349	0588	0845	1104	1359	1606	1843	2064	2267	2446	2593	2701	2756	2742	2633	2384	1897	0704
0.10	0438	0514	0696	0922	1162	1405	1643	1873	2089	2287	2461	2604	2707	2756	2735	2617	2353	1839	0432
0.15	0659	0711	0849	1039	1254	1479	1704	1923	2130	2320	2487	2622	2716	2756	2723	2588	2299	1732	
0.20	0881	0920	1029	1187	1375	1579	1787	1992	2187	2366	2521	2646	2728	2753	2703	2543	2214	1559	
0.25	1105	1136	1224	1356	1519	1700	1889	2077	2258	2422	2564	2674	2740	2746	2670	2475	2087	1275	
0.30	1331	1356	1429	1540	1680	1840	2008	2178	2341	2489	2613	2704	2749	2729	2619	2374	1895	0723	
0.35	1559	1579	1639	1733	1854	1992	2141	2290	2433	2561	2665	2732	2750	2696	2540	2222	1593		
0.40	1786	1803	1853	1933	2035	2154	2281	2409	2530	2635	2714	2752	2735	2636	2415	1987	1045		
0.45	2011	2025	2067	2133	2218	2318	2424	2530	2626	2704	2752	2755	2692	2531	2215	1597			
0.50	2229	2241	2275	2329	2399	2479	2563	2644	2713	2759	2769	2725	2600	2351	1880	0757			
0.55	2436	2445	2472	2513	2567	2627	2688	2741	2777	2784	2746	2639	2427	2035	1234				
0.60	2621	2628	2647	2676	2713	2751	2784	2804	2800	2757	2654	2457	2104	1422					
0.65	2772	2775	2786	2802	2819	2831	2831	2810	2753	2641	2441	2096	1446						
0.70	2866	2866	2867	2866	2859	2838	2796	2718	2585	2365	1996	1298							
0.75	2869	2865	2853	2830	2789	2723	2618	2452	2190	1753	0825								
0.80	2718	2708	2677	2620	2527	2385	2167	1820	1190										
0.85	2278	2256	2188	2063	1858	1519	0860												
0.90	0965	0880	0540																

 $\tau=90^\circ$ $\bar{\mu}=29^\circ$

r.l.u.	0.00	0.05	0.10	0.15	0.20	0.25	0.30	0.35	0.40	0.45	0.50	0.55	0.60	0.65	0.70	0.75	0.80	0.85	0.90	0.95
0.00	—	0258	0514	0768	1019	1265	1504	1735	1954	2159	2346	2510	2645	2743	2792	2778	2678	2455	2034	1167
0.05	0197	0322	0548	0791	1036	1278	1515	1743	1961	2165	2351	2514	2648	2744	2792	2776	2673	2446	2019	1130
0.10	0396	0469	0642	0857	1085	1317	1547	1770	1983	2183	2366	2525	2655	2748	2791	2770	2659	2421	1973	1010
0.15	0596	0646	0778	0960	1166	1382	1600	1814	2020	2214	2390	2544	2668	2754	2790	2758	2635	2376	1891	0757
0.20	0798	0836	0940	1093	1274	1471	1674	1876	2072	2257	2425	2571	2686	2762	2786	2740	2597	2307	1760	
0.25	1003	1033	1118	1246	1405	1582	1768	1955	2139	2312	2469	2604	2708	2771	2779	2713	2541	2206	1559	
0.30	1212	1236	1306	1415	1553	1710	1878	2050	2219	2379	2523	2643	2732	2778	2765	2671	2460	2058	1235	
0.35	1424	1444	1503	1596	1715	1854	2004	2159	2311	2455	2583	2687	2757	2780	2740	2609	2342	1839	0558	
0.40	1638	1655	1705	1785	1888	2009	2141	2278	2413	2538	2647	2730	2777	2772	2696	2514	2167	1489		
0.45	1855	1869	1911	1979	2067	2172	2286	2404	2519	2625	2711	2769	2786	2745	2620	2368	1896	0799		
0.50	2071	2083	2118	2175	2250	2338	2434	2533	2627	2708	2768	2796	2775	2686	2494	2135	1433			
0.55	2282	2292	2322	2369	2430	2502	2580	2657	2727	2781	2809	2797	2728	2572	2281	1741				
0.60	2485	2493	2516	2553	2601	2656	2713	2767	2808	2829	2817	2754	2617	2365	1909	0901				
0.65	2670	2675	2693	2719	2752	2789	2823	2848	2855	2834	2768	2636	2399	1983	1138					
0.70	2824	2827	2837	2852	2869	2883	2889	2879	2842	2764	2623	2384	1973	1159						
0.75	2927	2928	2930	2930	2926	2913	2882	2825	2727	2565	2303	1863	0954							
0.80	2949	2946	2936	2918	2886	2834	2752	2625	2428	2118	1591									
0.85	2833	2825	2799	2753	2678	2566	2397	2141	1730	0924										
0.90	2468	2450	2396	2298	2141	1898	1502	0677												
0.95	1493	1446	1292	0968																

5.3. Absorption Corrections

(a) Small Crystal bathed in Narrow Beam

The transmission factor $A(hkl)$ included in equations 5.2.4 (13), (14), (15) and (16) occurs when the intensity of any particular reflection from a crystal is affected by absorption in the crystal. If dV is a volume element in the crystal, and p and q are the lengths of the paths of the incident and reflected beams in the crystal, then the X-rays reflected by the crystal are reduced in intensity by the factor

$$\frac{1}{V} \int \exp\{-\mu(p+q)\} dV \quad \dots (1)$$

the integral being taken over that volume of the crystal which is bathed in X-rays. If the beam were not of uniform intensity, the expression would be more complicated.

The integral can be evaluated rigorously only for certain shapes of specimens. An evaluation of this transmission factor, which is *dimensionless*, is given in 5.3.5 and 5.3.6. A general discussion is also given in 5.3.7.

(b) Large Crystal or Crystalline Powder Block intercepting the Entire Narrow Beam

In this case, where ρ' instead of ρ is to be determined, the effect of absorption can be expressed by a quantity A_c , as follows:

$$\rho' = \frac{E\omega}{I} = QA_c \quad \dots (2)$$

A_c has the *dimensions* of *cm.* and is given by

$$\frac{1}{S_0} \int \exp\{-\mu(p+q)\} dV \quad \dots (3)$$

Values of A_c are given in 5.3.1, 5.3.2, 5.3.3 and 5.3.4.

5.3.1. Reflection of Narrow Beam from Planes Parallel to Extended Face of Crystal

(a) Crystal of Sufficient Thickness to give Negligible Transmission

If S is the area of the beam, the area of crystal irradiated is $S \operatorname{cosec} \theta$, and the volume element at a depth t has volume $dV = S \operatorname{cosec} \theta dt$.

Also $p = q = t \operatorname{cosec} \theta$.

Then

$$A_c = \int_0^\infty \exp\{-\mu(2t \operatorname{cosec} \theta)\} \operatorname{cosec} \theta dt = \frac{1}{2\mu} \quad \dots (4)$$

(b) Transmission not Negligible, Crystal Thickness t

$$A_c = \frac{1 - \exp\{-2\mu t \operatorname{cosec} \theta\}}{2\mu} \quad \dots (5)$$

5.3.2. Reflection from Crystal Planes inclined at Angle ϕ to Extended Face of Crystal Block of Negligible Transmission. The normal to the crystal face is in the plane of the incident and reflected beams.

$$A_c = \frac{1}{\mu} \left[\frac{1}{1 + \frac{\sin(\theta+\phi)}{\sin(\theta-\phi)}} \right] \quad \dots (6)$$

where the incident beam is at an angle $(\theta+\phi)$ to the crystal face.

5.3.3. Transmission when the Reflecting Planes are Perpendicular to the Surfaces of the Block, of Thickness t . The normal to the surfaces is in the plane of the incident and reflected beams.

All the paths, $p+q$, are equal to $t \sec \theta$ for a given value of θ , and thus

$$A_c = t \sec \theta \exp(-\mu t \sec \theta) \quad \dots (7)$$

5.3.4. Transmission when the Reflecting Planes are inclined at an Angle $(\pi/2) - \phi$ to the Surfaces of the Block of Thickness t . The normal to the surface is in the plane of the incident and reflected beams.

$$A_c = \frac{[\exp\{-\mu t \sec(\theta+\phi)\} - \exp\{-\mu t \sec(\theta-\phi)\}]}{\mu \left[1 - \frac{\sec(\theta+\phi)}{\sec(\theta-\phi)} \right]} \quad \dots (8)$$

The incident beam is at angle $(\theta-\phi)$ to the normal to the surface of the block.

5.3.5. Cylindrical Crystal of Radius R , bathed in a Uniform Beam of X-rays Normal to its Axis (W. L. Bond)

5.3.5.1. The 1935 *International Tables for the Determination of Crystal Structures* gave X-ray absorption correction tables based on Claassen's paper [23]. Claassen's method was a graphical one. Bradley [21] later developed a quasi-rigorous method for calculating the absorption in terms of μR (μ linear absorption coefficient, R radius of cylinder) which is reasonably accurate for $\mu R > 2$. Bradley's results were checked by graphical integration by Taylor and Sinclair [39].

To avoid the graphical approach one can use modern automatic computing methods. Consider a circular cross-section of the cylinder and a beam entering from the upper right at an angle θ to the y axis, being reflected from an element of volume about the point of co-ordinates R_x, R_y , then leaving towards the lower right, the deflection angle being 2θ . It is readily deduced that the path length P inside the circle is

$$P = R\sqrt{1 - (x \cos \theta - y \sin \theta)^2} + R\sqrt{1 - (x \cos \theta + y \sin \theta)^2} - 2xR \sin \theta \quad \dots (9)$$

For θ values of $0^\circ, 5^\circ, 10^\circ, \dots, 90^\circ$ and path lengths

5.3. ABSORPTION CORRECTIONS

0.1R, 0.2R, . . . , an I.B.M. card Programmed Electronic Calculator solved this equation and integrated to give the areas ΔS of the regions. If we attribute a mean path length l to each region the results are as in Table 5.3.5A. This gives ΔS and l for successive values of θ and hence the transmission factor $A = \sum e^{-\mu R l} \Delta S$. As an example of the use of this table consider the case $R=2$, $\theta=0$, $\mu=1$, for which

$$A = 0.00005e^{-2 \times 0.05} + 0.00037e^{-2 \times 0.15} + 0.0010e^{-2 \times 0.25} \\ + \dots + 0.3910e^{-2 \times 1.95}$$

It is often more convenient in use to replace the transmission factor A by the absorption factor $A^* = A^{-1}$, i.e. the number by which the apparent intensity should be multiplied to get the "true" intensity. In this way Table 5.3.5B has been prepared.

5.3.5.2. For large values of μR (>8) this method gives erroneous results, since almost all the reflection is from the zone of shortest path length and the "mean path length" concept is too crude for such a rapidly varying function. However, we can use series expansions as Claassen did, basing them on the values of ΔS given in Table 5.3.5A (using only the first few ΔS , since the penetration is small for large μR). We then write our series as

$$A = (A^*)^{-1} = a(\mu R)^{-1} + b(\mu R)^{-2} + \dots \quad (10)$$

Table 5.3.5C gives the values of the coefficients a , b , c , . . . for 5° intervals of θ . We can find A and hence A^* for intermediate values of θ by plotting A against $\sin^2 \theta$ (A. J. Bradley [21]). Note that for small θ values $a = 2\theta^2/3\pi$.

TABLE 5.3.5A (W. L. BOND)

NOTE: For recent and more accurate data for Tables 5.3.5 A and B, reference should be made to Weber, K. (1967), *Acta Cryst.*, **22**, —.

Data for Calculation of Transmission Factor A for Cylinder, Radius R , where $A = \sum e^{-\mu R l} \Delta S$
 ΔS and l Values for Successive Values of the Bragg Angle θ

$\theta=0^\circ$		$\theta=5^\circ$		$\theta=10^\circ$		$\theta=15^\circ$		$\theta=20^\circ$		$\theta=25^\circ$	
ΔS	l	ΔS	l	ΔS	l	ΔS	l	ΔS	l	ΔS	l
0.00005	0.05	0.0003	0.05	0.0009	0.05	0.0019	0.05	0.0031	0.05	0.0046	0.05
0.00037	0.15	0.0008	0.15	0.0016	0.15	0.0028	0.15	0.0042	0.15	0.0059	0.15
0.00102	0.25	0.0014	0.25	0.0025	0.25	0.0039	0.25	0.0055	0.25	0.0073	0.25
0.00200	0.35	0.0022	0.35	0.0035	0.35	0.0051	0.35	0.0069	0.35	0.0089	0.35
0.00332	0.45	0.0036	0.45	0.0046	0.45	0.0065	0.45	0.0084	0.45	0.0105	0.45
0.00502	0.55	0.0053	0.55	0.0060	0.55	0.0080	0.55	0.0101	0.55	0.0123	0.55
0.00713	0.65	0.0073	0.65	0.0076	0.65	0.0097	0.65	0.0119	0.65	0.0142	0.65
0.00968	0.75	0.0098	0.75	0.0104	0.75	0.0116	0.75	0.0139	0.75	0.0162	0.75
0.01273	0.85	0.0128	0.85	0.0132	0.85	0.0137	0.85	0.0161	0.85	0.0184	0.85
0.01635	0.95	0.0164	0.95	0.0166	0.95	0.0160	0.95	0.0185	0.95	0.0208	0.95
0.02065	1.05	0.0206	1.05	0.0206	1.05	0.0202	1.05	0.0212	1.05	0.0234	1.05
0.02577	1.15	0.0257	1.15	0.0254	1.15	0.0250	1.15	0.0241	1.15	0.0262	1.15
0.03191	1.25	0.0317	1.25	0.0311	1.25	0.0302	1.25	0.0274	1.25	0.0294	1.25
0.03939	1.35	0.0390	1.35	0.0381	1.35	0.0366	1.35	0.0333	1.35	0.0328	1.35
0.04869	1.45	0.0482	1.45	0.0466	1.45	0.0443	1.45	0.0414	1.45	0.0368	1.45
0.06068	1.55	0.0599	1.55	0.0576	1.55	0.0541	1.55	0.0498	1.55	0.0414	1.55
0.07698	1.65	0.0758	1.65	0.0723	1.65	0.0671	1.65	0.0607	1.65	0.0510	1.65
0.10138	1.75	0.0994	1.75	0.0939	1.75	0.0857	1.75	0.0759	1.75	0.0656	1.75
0.14587	1.85	0.1420	1.85	0.1311	1.85	0.1154	1.85	0.0996	1.85	0.0832	1.85
0.39101	1.95	0.3110	1.95	0.2458	1.95	0.1967	1.95	0.1519	1.95	0.1180	1.95
		0.0867	2.004	0.1703	2.015	0.2454	2.04	0.2437	2.05	0.1734	2.05
								0.0722	2.114	0.1867	2.15
										0.0129	2.203

5.3. ABSORPTION CORRECTIONS

TABLE 5.3.5A (continued)

Data for Calculation of Transmission Factor A for Cylinder, Radius R, where $A = \sum e^{-\mu R l} \Delta S$ ΔS and l Values for Successive Values of the Bragg Angle θ

$\theta=30^\circ$		$\theta=35^\circ$		$\theta=40^\circ$		$\theta=45^\circ$		$\theta=50^\circ$		$\theta=55^\circ$		$\theta=60^\circ$			
ΔS	l	ΔS	l	ΔS	l	ΔS	l	ΔS	l	ΔS	l	ΔS	l		
0.0063	0.05	0.0083	0.05	0.0105	0.05	0.0129	0.05	0.0153	0.05	0.0179	0.05	0.0204	0.05		
0.0078	0.15	0.0099	0.15	0.0121	0.15	0.0144	0.15	0.0169	0.15	0.0194	0.15	0.0217	0.15		
0.0093	0.25	0.0115	0.25	0.0137	0.25	0.0160	0.25	0.0184	0.25	0.0207	0.25	0.0230	0.25		
0.0110	0.35	0.0131	0.35	0.0154	0.35	0.0177	0.35	0.0199	0.35	0.0222	0.35	0.0243	0.35		
0.0127	0.45	0.0149	0.45	0.0171	0.45	0.0194	0.45	0.0215	0.45	0.0236	0.45	0.0256	0.45		
0.0145	0.55	0.0167	0.55	0.0189	0.55	0.0210	0.55	0.0231	0.55	0.0250	0.55	0.0267	0.55		
0.0164	0.65	0.0186	0.65	0.0207	0.65	0.0227	0.65	0.0246	0.65	0.0263	0.65	0.0279	0.65		
0.0185	0.75	0.0206	0.75	0.0226	0.75	0.0244	0.75	0.0261	0.75	0.0276	0.75	0.0289	0.75		
0.0206	0.85	0.0227	0.85	0.0245	0.85	0.0262	0.85	0.0277	0.85	0.0289	0.85	0.0300	0.85		
0.0229	0.95	0.0248	0.95	0.0265	0.95	0.0280	0.95	0.0292	0.95	0.0302	0.95	0.0310	0.95		
0.0254	1.05	0.0271	1.05	0.0286	1.05	0.0298	1.05	0.0308	1.05	0.0315	1.05	0.0319	1.05		
0.0280	1.15	0.0295	1.15	0.0307	1.15	0.0317	1.15	0.0323	1.15	0.0327	1.15	0.0328	1.15		
0.0309	1.25	0.0321	1.25	0.0330	1.25	0.0335	1.25	0.0338	1.25	0.0338	1.25	0.0335	1.25		
0.0341	1.35	0.0349	1.35	0.0353	1.35	0.0355	1.35	0.0353	1.35	0.0349	1.35	0.0342	1.35		
0.0376	1.45	0.0379	1.45	0.0378	1.45	0.0375	1.45	0.0368	1.45	0.0360	1.45	0.0348	1.45		
0.0416	1.55	0.0412	1.55	0.0405	1.55	0.0396	1.55	0.0383	1.55	0.0369	1.55	0.0353	1.55		
0.0462	1.65	0.0450	1.65	0.0435	1.65	0.0417	1.65	0.0398	1.65	0.0378	1.65	0.0356	1.65		
0.0519	1.75	0.0494	1.75	0.0468	1.75	0.0440	1.75	0.0413	1.75	0.0385	1.75	0.0356	1.75		
0.0595	1.85	0.0550	1.85	0.0506	1.85	0.0465	1.85	0.0426	1.85	0.0388	1.85	0.0355	1.85		
0.0880	1.95	0.0650	1.95	0.0559	1.95	0.0492	1.95	0.0436	1.95	0.0388	1.95	0.0352	1.95		
0.1243	2.05	0.0816	2.05	0.0626	2.05	0.0511	2.05	0.0437	2.05	0.0386	2.05	0.0349	2.05		
0.1318	2.15	0.0864	2.15	0.0637	2.15	0.0514	2.15	0.0435	2.15	0.0382	2.15	0.0345	2.15		
0.1468	2.25	0.0956	2.25	0.0650	2.25	0.0514	2.25	0.0432	2.25	0.0377	2.25	0.0340	2.25		
0.0140	2.305	0.1103	2.35	0.0664	2.35	0.0512	2.35	0.0426	2.35	0.0371	2.35	0.0333	2.35		
		0.0478	2.421	0.0685	2.45	0.0506	2.45	0.0418	2.45	0.0363	2.45	0.0326	2.45		
				0.0791	2.55	0.0495	2.55	0.0406	2.55	0.0352	2.55	0.0316	2.55		
				0.0097	2.605	0.0477	2.65	0.0389	2.65	0.0339	2.65	0.0306	2.65		
						0.0442	2.75	0.0367	2.75	0.0323	2.75	0.0293	2.75		
						0.0111	2.814	0.0333	2.85	0.0303	2.85	0.0278	2.85		
								0.0277	2.95	0.0277	2.95	0.0260	2.95		
								0.0106	3.032	0.0242	3.05	0.0240	3.05		
										0.0191	3.25	0.0214	3.15		
										0.0081	3.238	0.0181	3.25		
												0.0135	3.35		
												0.0045	3.432		

5.3. ABSORPTION CORRECTIONS

TABLE 5.3.5A (continued)

Data for Calculation of Transmission Factor A for Cylinder, Radius R, where $A = \sum e^{-\mu R l} \Delta S$
 ΔS and l Values for Successive Values of the Bragg Angle θ

$\theta=65^\circ$		$\theta=70^\circ$		$\theta=75^\circ$		$\theta=80^\circ$		$\theta=85^\circ$		$\theta=90^\circ$	
ΔS	l	ΔS	l	ΔS	l	ΔS	l	ΔS	l	ΔS	l
0.0230	0.05	0.0255	0.05	0.0278	0.05	0.0298	0.05	0.0313	0.05	0.03183	0.05
0.0243	0.15	0.0266	0.15	0.0285	0.15	0.0304	0.15	0.0314	0.15	0.03181	0.15
0.0253	0.25	0.0273	0.25	0.0291	0.25	0.0306	0.25	0.0315	0.25	0.03177	0.25
0.0263	0.35	0.0281	0.35	0.0297	0.35	0.0309	0.35	0.0316	0.35	0.03171	0.35
0.0273	0.45	0.0289	0.45	0.0302	0.45	0.0311	0.45	0.0315	0.45	0.03163	0.45
0.0283	0.55	0.0296	0.55	0.0307	0.55	0.0313	0.55	0.0315	0.55	0.03153	0.55
0.0292	0.65	0.0302	0.65	0.0310	0.65	0.0313	0.65	0.0314	0.65	0.03141	0.65
0.0300	0.75	0.0308	0.75	0.0313	0.75	0.0313	0.75	0.0313	0.75	0.03126	0.75
0.0308	0.85	0.0313	0.85	0.0314	0.85	0.0313	0.85	0.0311	0.85	0.03110	0.85
0.0315	0.95	0.0317	0.95	0.0315	0.95	0.0312	0.95	0.0310	0.95	0.03092	0.95
0.0321	1.05	0.0320	1.05	0.0315	1.05	0.0311	1.05	0.0308	1.05	0.03071	1.05
0.0326	1.15	0.0321	1.15	0.0314	1.15	0.0309	1.15	0.0306	1.15	0.03049	1.15
0.0330	1.25	0.0322	1.25	0.0313	1.25	0.0307	1.25	0.0303	1.25	0.03024	1.25
0.0333	1.35	0.0322	1.35	0.0312	1.35	0.0305	1.35	0.0301	1.35	0.02996	1.35
0.0335	1.45	0.0321	1.45	0.0310	1.45	0.0302	1.45	0.0298	1.45	0.02967	1.45
0.0335	1.55	0.0319	1.55	0.0307	1.55	0.0299	1.55	0.0295	1.55	0.02934	1.55
0.0334	1.65	0.0317	1.65	0.0305	1.65	0.0296	1.65	0.0291	1.65	0.02899	1.65
0.0332	1.75	0.0314	1.75	0.0301	1.75	0.0293	1.75	0.0288	1.75	0.02862	1.75
0.0330	1.85	0.0311	1.85	0.0298	1.85	0.0289	1.85	0.0284	1.85	0.02822	1.85
0.0326	1.95	0.0307	1.95	0.0294	1.95	0.0285	1.95	0.0280	1.95	0.02779	1.95
0.0322	2.05	0.0303	2.05	0.0289	2.05	0.0280	2.05	0.0275	2.05	0.02733	2.05
0.0318	2.15	0.0298	2.15	0.0285	2.15	0.0275	2.15	0.0270	2.15	0.02684	2.15
0.0312	2.25	0.0293	2.25	0.0279	2.25	0.0270	2.25	0.0265	2.25	0.02632	2.25
0.0306	2.35	0.0287	2.35	0.0273	2.35	0.0264	2.35	0.0259	2.35	0.02576	2.35
0.0299	2.45	0.0280	2.45	0.0267	2.45	0.0258	2.45	0.0253	2.45	0.02516	2.45
0.0291	2.55	0.0273	2.55	0.0260	2.55	0.0251	2.55	0.0247	2.55	0.02452	2.55
0.0281	2.65	0.0264	2.65	0.0252	2.65	0.0244	2.65	0.0240	2.65	0.02384	2.65
0.0271	2.75	0.0255	2.75	0.0244	2.75	0.0237	2.75	0.0232	2.75	0.02311	2.75
0.0259	2.85	0.0245	2.85	0.0235	2.85	0.0228	2.85	0.0225	2.85	0.02233	2.85
0.0246	2.95	0.0234	2.95	0.0226	2.95	0.0219	2.95	0.0216	2.95	0.02150	2.95
0.0230	3.05	0.0222	3.05	0.0215	3.05	0.0210	3.05	0.0207	3.05	0.02059	3.05
0.0213	3.15	0.0208	3.15	0.0203	3.15	0.0199	3.15	0.0197	3.15	0.01961	3.15
0.0192	3.25	0.0192	3.25	0.0190	3.25	0.0188	3.25	0.0186	3.25	0.01855	3.25
0.0167	3.35	0.0174	3.35	0.0175	3.35	0.0175	3.35	0.0174	3.35	0.01739	3.35
0.0135	3.45	0.0153	3.45	0.0158	3.45	0.0160	3.45	0.0161	3.45	0.01610	3.45
0.0088	3.55	0.0127	3.55	0.0139	3.55	0.0144	3.55	0.0146	3.55	0.01466	3.55
0.0009	3.613	0.0092	3.65	0.0116	3.65	0.0125	3.65	0.0129	3.65	0.01301	3.65
		0.0027	3.729	0.0085	3.75	0.0102	3.75	0.0109	3.75	0.01106	3.75
				0.0027	3.832	0.0070	3.85	0.0082	3.85	0.00859	3.85
						0.0012	3.920	0.0037	3.942	0.00473	3.95

TABLE 5.3.5B
(W. L. BOND)
Absorption Correction Factors A* for Successive Values of θ
Cylinders, Radius R

μR	0°	5°	10°	15°	20°	25°	30°	35°	40°	μR
0	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	0
0.1	1.18	1.18	1.18	1.18	1.18	1.18	1.18	1.18	1.18	0.1
0.2	1.40	1.40	1.40	1.40	1.40	1.40	1.39	1.39	1.39	0.2
0.3	1.65	1.65	1.65	1.65	1.65	1.64	1.64	1.63	1.63	0.3
0.4	1.95	1.95	1.95	1.94	1.94	1.93	1.92	1.91	1.90	0.4
0.5	2.29	2.29	2.29	2.28	2.27	2.26	2.24	2.22	2.20	0.5
0.6	2.69	2.69	2.69	2.67	2.65	2.63	2.60	2.57	2.53	0.6
0.7	3.16	3.16	3.15	3.13	3.09	3.05	3.01	2.96	2.91	0.7
0.8	3.70	3.70	3.68	3.65	3.60	3.54	3.47	3.39	3.32	0.8
0.9	4.33	4.33	4.30	4.24	4.17	4.08	3.98	3.87	3.76	0.9
1.0	5.06	5.05	5.01	4.92	4.81	4.68	4.54	4.39	4.24	1.0
1.1	5.90	5.88	5.81	5.69	5.54	5.36	5.16	4.96	4.76	1.1
1.2	6.86	6.84	6.74	6.57	6.35	6.10	5.84	5.57	5.32	1.2
1.3	7.96	7.93	7.79	7.55	7.25	6.92	6.58	6.23	5.91	1.3
1.4	9.23	9.18	8.97	8.65	8.25	7.82	7.37	6.94	6.53	1.4
1.5	10.7	10.6	10.3	9.88	9.35	8.79	8.22	7.68	7.19	1.5
1.6	12.3	12.2	11.8	11.2	10.6	9.84	9.13	8.47	7.87	1.6
1.7	14.2	14.0	13.5	12.7	11.9	11.0	10.1	9.30	8.58	1.7
1.8	16.3	16.0	15.4	14.4	13.3	12.2	11.1	10.2	9.32	1.8
1.9	18.6	18.3	17.5	16.2	14.8	13.5	12.2	11.1	10.1	1.9
2.0	21.3	20.9	19.8	18.2	16.5	14.8	13.3	12.0	10.9	2.0
2.1	24.2	23.7	22.3	20.3	18.2	16.2	14.5	12.9	11.7	2.1
2.2	27.5	26.9	25.1	22.6	20.1	17.7	15.7	13.9	12.5	2.2
2.3	31.2	30.4	28.1	25.1	22.0	19.3	16.9	14.9	13.3	2.3
2.4	35.3	34.2	31.4	27.7	24.1	20.9	18.2	16.0	14.2	2.4
2.5	39.8	38.5	34.9	30.5	26.2	22.5	19.5	17.0	15.0	2.5
2.6	44.7	43.1	38.7	33.4	28.5	24.2	20.8	18.1	15.9	2.6
2.7	50.1	48.1	42.8	36.5	30.8	26.0	22.2	19.2	16.8	2.7
2.8	56.1	53.5	47.2	39.7	33.2	27.8	23.6	20.3	17.7	2.8
2.9	62.5	59.4	51.8	43.1	35.7	29.6	25.0	21.4	18.6	2.9
3.0	69.5	65.8	56.7	46.6	38.2	31.5	26.4	22.5	19.5	3.0
3.1	77.2	72.6	61.8	50.3	40.8	33.4	27.9	23.7	20.4	3.1
3.2	85.4	79.9	67.3	54.0	43.5	35.4	29.3	24.8	21.4	3.2
3.3	94.2	87.6	72.9	57.9	46.2	37.3	30.8	26.0	22.3	3.3
3.4	104	95.9	78.9	61.9	48.9	39.3	32.3	27.1	23.2	3.4
3.5	114	105	85.0	65.9	51.7	41.3	33.8	28.3	24.2	3.5
3.6	125	114	91.4	70.1	54.6	43.3	35.3	29.5	25.1	3.6
3.7	136	124	98.0	74.4	57.4	45.4	36.9	30.7	26.1	3.7
3.8	149	134	105	78.7	60.4	47.5	38.4	31.9	27.0	3.8
3.9	162	145	112	83.1	63.3	49.5	39.9	33.1	28.0	3.9
4.0	175	156	119	87.6	66.3	51.6	41.5	34.3	28.9	4.0
4.1	190	168	127	92.1	69.3	53.8	43.1	35.5	29.9	4.1
4.2	206	180	134	96.7	72.3	55.9	44.6	36.7	30.9	4.2
4.3	222	193	142	101	75.4	58.0	46.2	37.9	31.8	4.3
4.4	239	206	150	106	78.5	60.2	47.8	39.1	32.8	4.4

TABLE 5.3.5B (continued)
Absorption Correction Factors A* for Successive Values of θ
Cylinders, Radius R

μR	0°	5°	10°	15°	20°	25°	30°	35°	40°	μR
4.5	257	220	158	111	81.6	62.3	49.4	40.4	33.8	4.5
4.6	275	234	166	116	84.7	64.5	51.0	41.6	34.8	4.6
4.7	295	249	175	121	87.8	66.7	52.6	42.8	35.8	4.7
4.8	316	264	183	125	91.0	68.9	54.2	44.1	36.7	4.8
4.9	337	280	192	130	94.2	71.1	55.8	45.3	37.7	4.9
5.0	359	296	200	135	97.4	73.3	57.5	46.6	38.7	5.0
5.1	383	313	209	140	101	75.5	59.1	47.8	39.7	5.1
5.2	407	330	218	145	104	77.8	60.7	49.1	40.7	5.2
5.3	432	348	228	150	107	80.0	62.4	50.3	41.7	5.3
5.4	458	366	237	156	110	82.3	64.0	51.6	42.7	5.4
5.5	485	384	246	161	114	84.5	65.7	52.9	43.7	5.5
5.6	513	403	255	166	117	86.8	67.3	54.1	44.7	5.6
5.7	542	422	265	171	120	89.1	69.0	55.4	45.7	5.7
5.8	573	442	275	176	124	91.4	70.7	56.7	46.8	5.8
5.9	604	462	284	182	127	93.6	72.4	58.0	47.8	5.9
6.0	636	483	294	187	130	95.9	74.0	59.2	48.8	6.0
6.1	670	504	304	192	134	98.3	75.7	60.5	49.8	6.1
6.2	704	525	314	198	137	101	77.4	61.8	50.8	6.2
6.3	740	547	324	203	140	103	79.1	63.1	51.9	6.3
6.4	777	569	334	209	144	105	80.8	64.4	52.9	6.4
6.5	814	591	345	214	147	108	82.5	65.7	53.9	6.5
6.6	853	614	355	219	151	110	84.2	67.0	54.9	6.6
6.7	894	638	365	225	154	112	85.9	68.3	56.0	6.7
6.8	935	661	376	231	158	115	87.6	69.6	57.0	6.8
6.9	978	685	386	236	161	117	89.4	70.9	58.0	6.9
7.0	1022	710	397	242	165	119	91.1	72.2	59.1	7.0
7.1	1067	735	408	247	168	122	92.8	73.6	60.1	7.1
7.2	1113	760	418	253	172	124	94.6	74.9	61.2	7.2
7.3	1161	785	429	259	175	127	96.3	76.2	62.2	7.3
7.4	1210	811	440	264	179	129	98.1	77.5	63.3	7.4
7.5	1260	837	451	270	182	131	99.8	78.9	64.3	7.5
7.6	1311	864	462	276	186	134	102	80.2	65.4	7.6
7.7	1364	891	473	281	190	136	103	81.5	66.4	7.7
7.8	1418	918	484	287	193	139	105	82.9	67.5	7.8
7.9	1474	945	495	293	197	141	107	84.2	68.5	7.9
8.0	1530	974	507	299	200	144	109	85.5	69.6	8.0
9.0	2200	1270	623	357	236	167	126	98.1	79.6	9.0
10.0	3050	1600	743	417	272	191	143	111	89.7	10.0
11.0	4080	1950	868	478	308	215	160	124	99.7	11.0
12.0	5320	2320	995	541	345	240	178	137	110	12.0
13.0	6790	2710	1130	604	381	264	195	150	120	13.0
14.0	8500	3110	1260	667	419	289	212	163	130	14.0
15.0	10500	3530	1400	731	457	313	230	176	140	15.0
16.0	12700	3970	1540	795	495	338	247	189	151	16.0
17.0	15300	4410	1675	860	533	362	265	203	161	17.0
18.0	18200	4860	1820	925	572	387	282	216	171	18.0
19.0	21400	5320	1960	991	610	412	300	229	181	19.0
20.0	25000	5790	2100	1060	649	438	317	242	192	20.0

TABLE 5.3.5B (continued)
Absorption Correction Factors A* for Successive Values of θ
Cylinders, Radius R

μR	45°	50°	55°	60°	65°	70°	75°	80°	85°	90°	μR
0	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	0
0.1	1.18	1.18	1.18	1.18	1.18	1.18	1.18	1.18	1.18	1.18	0.1
0.2	1.39	1.39	1.38	1.38	1.38	1.38	1.38	1.37	1.37	1.37	0.2
0.3	1.62	1.62	1.61	1.61	1.60	1.59	1.59	1.59	1.59	1.59	0.3
0.4	1.89	1.87	1.86	1.85	1.84	1.83	1.82	1.82	1.81	1.81	0.4
0.5	2.18	2.16	2.13	2.12	2.10	2.08	2.07	2.06	2.05	2.05	0.5
0.6	2.50	2.47	2.43	2.40	2.37	2.35	2.33	2.31	2.30	2.30	0.6
0.7	2.85	2.80	2.75	2.71	2.66	2.63	2.60	2.58	2.56	2.56	0.7
0.8	3.24	3.16	3.09	3.03	2.97	2.92	2.88	2.85	2.84	2.83	0.8
0.9	3.65	3.55	3.46	3.37	3.29	3.23	3.18	3.14	3.11	3.11	0.9
1.0	4.10	3.97	3.84	3.73	3.63	3.55	3.48	3.43	3.40	3.39	1.0
1.1	4.58	4.40	4.24	4.10	3.97	3.87	3.79	3.73	3.69	3.68	1.1
1.2	5.08	4.86	4.66	4.49	4.33	4.20	4.11	4.03	3.98	3.97	1.2
1.3	5.61	5.34	5.09	4.88	4.70	4.54	4.43	4.34	4.28	4.27	1.3
1.4	6.16	5.83	5.54	5.29	5.07	4.89	4.75	4.65	4.58	4.57	1.4
1.5	6.74	6.35	6.00	5.71	5.45	5.24	5.08	4.96	4.89	4.87	1.5
1.6	7.34	6.87	6.47	6.13	5.84	5.60	5.42	5.28	5.19	5.17	1.6
1.7	7.96	7.42	6.95	6.57	6.23	5.96	5.75	5.60	5.50	5.48	1.7
1.8	8.59	7.97	7.45	7.01	6.63	6.33	6.09	5.92	5.81	5.78	1.8
1.9	9.25	8.54	7.94	7.45	7.03	6.69	6.44	6.24	6.12	6.09	1.9
2.0	9.91	9.12	8.45	7.91	7.44	7.06	6.78	6.56	6.43	6.40	2.0
2.1	10.6	9.71	8.97	8.36	7.84	7.44	7.13	6.89	6.75	6.71	2.1
2.2	11.3	10.3	9.49	8.82	8.26	7.81	7.47	7.22	7.06	7.02	2.2
2.3	12.0	10.9	10.0	9.29	8.67	8.19	7.82	7.54	7.38	7.33	2.3
2.4	12.7	11.5	10.5	9.76	9.09	8.57	8.17	7.87	7.69	7.64	2.4
2.5	13.4	12.1	11.1	10.2	9.51	8.95	8.53	8.20	8.01	7.96	2.5
2.6	14.2	12.8	11.6	10.7	9.93	9.33	8.88	8.53	8.33	8.27	2.6
2.7	14.9	13.4	12.2	11.2	10.4	9.72	9.23	8.87	8.64	8.58	2.7
2.8	15.6	14.0	12.7	11.7	10.8	10.1	9.59	9.20	8.96	8.90	2.8
2.9	16.4	14.6	13.2	12.1	11.2	10.5	9.95	9.53	9.28	9.21	2.9
3.0	17.1	15.3	13.8	12.6	11.6	10.9	10.3	9.86	9.60	9.53	3.0
3.1	17.9	15.9	14.3	13.1	12.1	11.3	10.7	10.2	9.92	9.84	3.1
3.2	18.7	16.6	14.9	13.6	12.5	11.7	11.0	10.5	10.2	10.2	3.2
3.3	19.4	17.2	15.5	14.1	12.9	12.0	11.4	10.9	10.6	10.5	3.3
3.4	20.2	17.9	16.0	14.6	13.4	12.4	11.7	11.2	10.9	10.8	3.4
3.5	21.0	18.5	16.6	15.1	13.8	12.8	12.1	11.5	11.2	11.1	3.5
3.6	21.7	19.2	17.1	15.6	14.2	13.2	12.5	11.9	11.5	11.4	3.6
3.7	22.5	19.8	17.7	16.1	14.7	13.6	12.8	12.2	11.8	11.7	3.7
3.8	23.3	20.5	18.3	16.6	15.1	14.0	13.2	12.6	12.2	12.1	3.8
3.9	24.1	21.2	18.8	17.1	15.6	14.4	13.6	12.9	12.5	12.4	3.9
4.0	24.9	21.8	19.4	17.6	16.0	14.8	13.9	13.2	12.8	12.7	4.0
4.1	25.7	22.5	20.0	18.1	16.4	15.2	14.3	13.6	13.1	13.0	4.1
4.2	26.5	23.2	20.6	18.6	16.9	15.6	14.6	13.9	13.5	13.3	4.2
4.3	27.3	23.8	21.1	19.1	17.3	16.0	15.0	14.3	13.8	13.7	4.3
4.4	28.1	24.5	21.7	19.6	17.8	16.4	15.4	14.6	14.1	14.0	4.4

TABLE 5.3.5B (continued)
Absorption Correction Factors A* for Successive Values of θ
Cylinders, Radius R

μR	45°	50°	55°	60°	65°	70°	75°	80°	85°	90°	μR
4.5	28.9	25.2	22.3	20.1	18.2	16.8	15.7	14.9	14.4	14.3	4.5
4.6	29.7	25.8	22.9	20.6	18.7	17.2	16.1	15.3	14.8	14.6	4.6
4.7	30.5	26.5	23.4	21.1	19.1	17.6	16.5	15.6	15.1	14.9	4.7
4.8	31.3	27.2	24.0	21.6	19.6	18.0	16.9	16.0	15.4	15.3	4.8
4.9	32.1	27.9	24.6	22.1	20.0	18.4	17.2	16.3	15.7	15.6	4.9
5.0	32.9	28.6	25.2	22.6	20.5	18.8	17.6	16.7	16.1	15.9	5.0
5.1	33.7	29.2	25.8	23.1	20.9	19.2	18.0	17.0	16.4	16.2	5.1
5.2	34.5	29.9	26.3	23.6	21.4	19.6	18.3	17.3	16.7	16.6	5.2
5.3	35.3	30.6	26.9	24.1	21.8	20.0	18.7	17.7	17.1	16.9	5.3
5.4	36.1	31.3	27.5	24.6	22.3	20.4	19.1	18.0	17.4	17.2	5.4
5.5	37.0	32.0	28.1	25.2	22.7	20.9	19.5	18.4	17.7	17.5	5.5
5.6	37.8	32.7	28.7	25.7	23.2	21.3	19.8	18.7	18.0	17.9	5.6
5.7	38.6	33.4	29.3	26.2	23.6	21.7	20.2	19.1	18.4	18.2	5.7
5.8	39.4	34.0	29.9	26.7	24.1	22.1	20.6	19.4	18.7	18.5	5.8
5.9	40.3	34.7	30.5	27.2	24.5	22.5	21.0	19.8	19.0	18.8	5.9
6.0	41.1	35.4	31.0	27.7	25.0	22.9	21.3	20.1	19.4	19.2	6.0
6.1	41.9	36.1	31.6	28.3	25.4	23.3	21.7	20.5	19.7	19.5	6.1
6.2	42.7	36.8	32.2	28.8	25.9	23.7	22.1	20.8	20.0	19.8	6.2
6.3	43.6	37.5	32.8	29.3	26.4	24.1	22.5	21.2	20.4	20.2	6.3
6.4	44.4	38.2	33.4	29.8	26.8	24.6	22.8	21.5	20.7	20.5	6.4
6.5	45.2	38.9	34.0	30.3	27.3	25.0	23.2	21.9	21.0	20.8	6.5
6.6	46.1	39.6	34.6	30.9	27.7	25.4	23.6	22.2	21.4	21.1	6.6
6.7	46.9	40.3	35.2	31.4	28.2	25.8	24.0	22.6	21.7	21.5	6.7
6.8	47.8	41.0	35.8	31.9	28.7	26.2	24.4	23.0	22.1	21.8	6.8
6.9	48.6	41.7	36.4	32.4	29.1	26.6	24.8	23.3	22.4	22.1	6.9
7.0	49.4	42.4	37.0	33.0	29.6	27.0	25.1	23.7	22.7	22.5	7.0
7.1	50.3	43.1	37.6	33.5	30.1	27.5	25.5	24.0	23.1	22.8	7.1
7.2	51.1	43.8	38.2	34.0	30.5	27.9	25.9	24.4	23.4	23.1	7.2
7.3	52.0	44.6	38.8	34.6	31.0	28.3	26.3	24.7	23.8	23.5	7.3
7.4	52.8	45.3	39.5	35.1	31.5	28.7	26.7	25.1	24.1	23.8	7.4
7.5	53.7	46.0	40.1	35.6	31.9	29.2	27.1	25.5	24.4	24.1	7.5
7.6	54.5	46.7	40.7	36.1	32.4	29.6	27.4	25.8	24.8	24.5	7.6
7.7	55.4	47.4	41.3	36.7	32.9	30.0	27.8	26.2	25.1	24.8	7.7
7.8	56.2	48.1	41.9	37.2	33.3	30.4	28.2	26.5	25.5	25.2	7.8
7.9	57.1	48.9	42.5	37.8	33.8	30.8	28.6	26.9	25.8	25.5	7.9
8.0	58.0	49.5	43.1	38.3	34.3	31.3	29.0	27.3	26.1	25.8	8.0
9.0	65.6	56.3	48.7	43.2	38.6	35.2	32.5	30.6	29.2	28.9	9.0
10.0	74.2	63.0	54.3	48.2	43.0	39.1	36.1	33.9	32.4	31.9	10.0
11.0	82.4	69.8	60.0	53.2	47.4	43.1	39.7	37.3	35.5	35.0	11.0
12.0	90.6	76.5	65.6	58.2	51.7	47.0	43.3	40.6	38.7	38.1	12.0
13.0	98.8	83.4	71.3	63.2	56.1	50.9	46.9	43.9	41.9	41.2	13.0
14.0	107	90.1	77.0	68.2	60.5	54.9	50.5	47.2	45.1	44.3	14.0
15.0	115	97.0	82.7	73.2	64.8	58.8	54.1	50.6	48.3	47.5	15.0
16.0	124	104	88.4	78.2	69.2	62.8	57.7	54.0	51.5	50.6	16.0
17.0	132	111	94.0	83.2	73.6	66.8	61.3	57.3	54.6	53.7	17.0
18.0	140	118	99.7	88.2	78.0	70.7	64.9	60.7	57.8	56.8	18.0
19.0	148	124	105	93.2	82.4	74.7	68.5	64.1	61.0	60.0	19.0
20.0	157	131	111	98.4	86.8	78.7	72.3	67.6	64.3	63.1	20.0

TABLE 5.3.5C

Alternative Method of Calculating Transmission Factor A for Cylinder, Radius R, where
 $A=(A^*)^{-1}=a(\mu R)^{-1}+b(\mu R)^{-2}+\dots$

$\theta \backslash i$	a	b	c	d	e	f	g
0	0	0	0.3183	0	0.955	0	7.1
5	0.001615	0.0314	0.0648	0.835	0.14		
10	0.00642	0.053	0.179	0.057			
15	0.01442	0.086	0.061	0.33			
20	0.0254	0.105	0.080	0.13			
25	0.0394	0.123	0.073	-0.16			
30	0.0560	0.139	0				
35	0.0752	0.150	-0.022				
40	0.0966	0.159	-0.10				
45	0.1199	0.164	-0.16				
50	0.1448	0.16	-0.20				
55	0.1741	0.13	-0.30				
60	0.1984	0.11	-0.21				
65	0.226	0.10	-0.33				
70	0.250	0.105	-0.48				
75	0.274	0.08	-0.52				
80	0.295	0.064	-0.64				
85	0.3107	0.03	-0.5				
90	0.3183	0	-0.53				

5.3.5.3. UPPER LEVELS OF EQUI-INCLINATION
WEISSENBERG PHOTOGRAPHS

A proper absorption correction can be made for upper levels of equi-inclination Weissenberg photographs by using $\mu \sec \nu$ in place of μ , and $Y/2$ in place of θ for compiling the tables. Here

$$\sin Y/2 = \sec \nu \sqrt{(\sin^2 \theta - \sin^2 \nu)}$$

(from Section 4.3.2 (4), (8), (9), pp. 176, 177).

Finally, the irradiated volume is greater for larger values of ν by the factor $\sec \nu$, and this should be allowed for by multiplying the resulting correction factor by $\cos \nu$. Hence the resulting correction factor is

$$\bar{A}^* = \cos \nu \{A^*(\mu R \sec \nu, Y/2)\} \dots (11)$$

Here ν is the angle between the generator of the given layer line and the equatorial plane (normal to the rotation axis); and Y is the angle between the projections of the incident and diffracted beams on to the equatorial plane.

5.3.5.4. OPTIMUM SIZE OF A CYLINDER

Plots of $(\mu R)^2/A^*$ show that for $\theta=0$ the optimum cylinder radius is that for which $\mu R=1.35$; for $\theta=10^\circ$ it is given by $\mu R=1.45$ and for $\theta=20^\circ$ it is given by

$\mu R=1.9$. Above $\theta=25^\circ$ there is no optimum, since $(\mu R)^2/A^*$ rises continuously from $\mu R=0$ to $\mu R=\infty$ if $\theta>25^\circ$. Hence a practical optimum radius for cylinders is that for which $\mu R=1.5$.

5.3.6. Sphere of Radius R, bathed in a Uniform Incident X-ray Beam (W. L. Bond)

A machine integration of

$$A = \frac{1}{\text{Vol}} \iiint e^{-\mu(p+q)} dx dy dz \dots (12)$$

throughout the sphere gives the results of Table 5:3.6A. It is worth noting that for $\theta=0^\circ$ and for $\theta=90^\circ$ the equation is integrable. For $\theta=0^\circ$ the transmission factor is

$$A = \frac{3}{2(\mu R)^3} \left\{ \frac{1}{2} - e^{-2\mu R} \left[\frac{1}{2} + \mu R + (\mu R)^2 \right] \right\} \dots (13)$$

while for $\theta=90^\circ$

$$A = \frac{3}{4\mu R} \left\{ \frac{1}{2} - \frac{1}{16(\mu R)^2} [1 - (1 + 4\mu R)e^{-4\mu R}] \right\} \dots (14)$$

Table 5.3.6B (p. 302) has been produced by interpolation from Table 5.3.6A.

TABLE 5.3.6A
Transmission Factor A for Sphere, Radius R, where

$$A = \frac{1}{V} \iiint e^{-\mu(p+q)} dx dy dz$$

μR	$\theta = 0^\circ$	15°	30°	45°	60°	75°	90°
0							
0.5	0.48181	0.48432	0.49166	0.50249	0.51424	0.52359	0.52725
1	0.24249	0.24812	0.26372	0.28532	0.30775	0.32541	0.33242
2	0.07142	0.07941	0.09967	0.12562	0.15183	0.17289	0.18166
3	0.02606	0.03350	0.05125	0.07343	0.09610	0.11498	0.12326
4	0.01156	0.01785	0.03228	0.05039	0.06932	0.08557	0.09302
5	0.005983	0.01122	0.02297	0.03795	0.05393	0.06796	0.07462
6	0.003470	0.007865	0.01762	0.03029	0.04403	0.05630	0.06228
7	0.002186	0.005924	0.01420	0.02513	0.03715	0.04801	0.05343
8	0.001465	0.004691	0.01185	0.02145	0.03211	0.04184	0.04678
9	0.001029	0.003851	0.01014	0.01869	0.02826	0.03706	0.04160
10	0.0007499	0.003249	0.008854	0.01654	0.02563	0.03326	0.03745

5.3.6.1. OPTIMUM SIZE OF SPHERES

Plotting $(\mu R)^3/A^*$ shows that there is no optimum size for spheres, since the total reflected energy decreases continuously from $\mu R=0$ to $\mu R=\infty$ for all values of θ .

The concept of "optimum size" is misleading. The most desirable condition is that the correction factor for $\theta=0^\circ$ be not too different from the correction factor for $\theta=90^\circ$. This is met if $\mu R < 2$, when the ratio of front to back factors is less than 2.6.

5.3.7. Crystal of Any Shape, bathed in Uniform Beam of X-rays (A. Hargreaves)

The expression to be evaluated is

$$A = \frac{\int_V \exp(-\mu x) dV}{V} \quad \dots (15)$$

where x is the path length in the crystal of the rays reflected from an element dV , and V is the volume of the crystal. Graphical methods for evaluating the integral are described by Hendershot [32], Albrecht [20] and Howells [33]; none of them is completely general.

Albrecht's method will be considered when applied to zero-layer-line reflections in an oscillation photograph of a crystal with a cross-section which is constant when viewed along the oscillation axis. If the specimen is divided into small volume elements we may write the approximate solution

$$A \simeq \frac{\sum_i \exp(-\mu x_i)}{n} \quad \dots (16)$$

where n is the number of elements. Let the incident

beam S_0 and the diffracted beam S be divided into a number of equally spaced rays (Fig. 5.3.7), and let the intersection of each pair of ray lines represent the centre of a projected volume element. Then the sum of

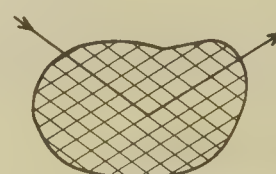


Fig. 5.3.7

the lengths in the crystal of each pair of intersecting ray lines gives the path length in the crystal of the beam diffracted by the associated volume element. Expression (16) may be evaluated by measuring, on a scale diagram, the path length x_i for each element, obtaining $e^{-\mu x_i}$ from an exponential table and then dividing $\sum e^{-\mu x_i}$ by n , the number of ray intersections within the cross-section of the crystal. It is unnecessary to draw new ray lines for each reflection if parallel lines are ruled on two pieces of celluloid. The celluloid masks are laid over the scale drawing of the crystal section in orientations determined by the directions of the incident and diffracted rays appropriate for the reflection under consideration.

Values of $\exp(-\mu x)$ may be obtained from Table 8.1 for the exponential function.

If the cross-section of the crystal is not constant when viewed along the oscillation axis it is necessary to repeat the above process for a number of layers. The number of layers and the number of rays in each layer are determined by the degree of accuracy required.

The computations for non-zero layer lines would, in general, be unduly laborious. For equi-inclination Weissenberg photographs, however, it is only necessary to increase the path of each ray by $\text{cosec } \nu$, where

ν is the inclination of the incident beam to the axis of rotation of the crystal; the increase can be effected by an appropriate change in the scale of the drawing of the cross-section of the crystal. The anti-equi-inclination method can be used to *eliminate* absorption corrections for needle-shaped and platy crystals (Kartha [12]).

Howells' method, which is a development of that described by Hendershot, enables equation 5.3(1) to be integrated by a semi-graphical procedure after dividing the crystal into a small number of suitable areas. The number of areas to be considered increases with the number of faces of the crystal; the faces are assumed to be flat. For crystals bounded by a small number of faces and when moderate or high accuracy is required, less computation is needed than in Albrecht's method, particularly in the case of crystals of high absorbing power. Howells' method is applicable to zero and non-zero layer lines in oscillation photographs and can also be used for equi-inclination Weissenberg photographs. In general, the method is not applicable to crystals for which the cross-section is not constant when viewed along the oscillation axis. It has, however, been extended by Howells to cover zero-layer-line reflections in two special cases of crystals of varying cross-section, viz. (a) that of a pyramidal form, and (b) that of a needle with its length perpendicular to the rotation axis.

Several recent papers have appeared on the subject of correction factors in crystals having fairly general shapes. Improved graphical methods have been described by Joel, Vera and Garaycochea [34] and by Rogers and Moffett [35]. Numerical methods have been developed by Grdenić [29] [30; with correction, 31] and by H. T. Evans [27]. An important development is the high-speed evaluation of transmission or absorption factors by means of electronic computers: see, for example, Busing and Levy [22].

5.3.8. Absorption Corrections in X-ray Examinations of Preferred Orientation in Flat Sheet Specimens (B. F. Decker)

The quantity required is a measure of the variation in diffracting volume and absorption for rays diffracted to different points in a given diffraction ring.

There are two expressions for the transmission factor: one is used when the diffracted rays leave the sheet at the face opposite to that entered by the incident beam, the transmission case, illustrated in Fig. 5.3.8(1); the other is used when the diffracted rays emerge from the face at which the incident beam enters the sheet, the reflection case. Custers [24] has evaluated both these expressions, but in a form which is unnecessarily complex. An expression for the transmission case has been derived by Decker [25] and Smoluchowski and Turner [37]. The form given by Decker is repeated here (with correction of an error in the original paper),

and an extension of the same treatment has led to the expression given for the reflection case.

In conjunction with the widespread use of counters to measure X-ray intensity in preferred orientation studies it has been found that two special cases are the most useful in practice. Accordingly these special

(Continued on page 306)

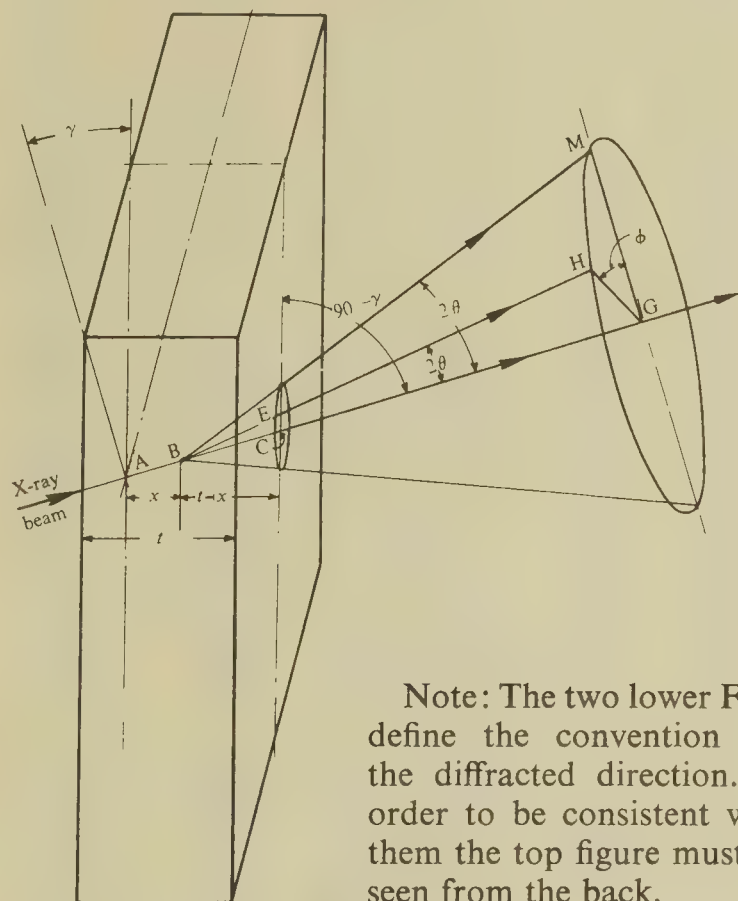


Fig. 5.3.8(1)

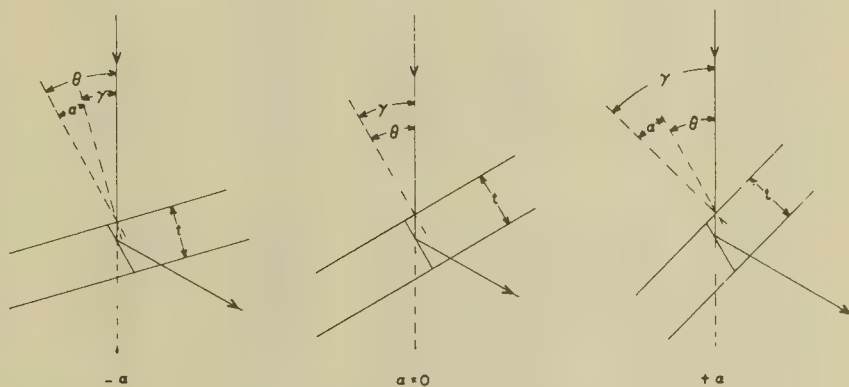


Fig. 5.3.8(2)

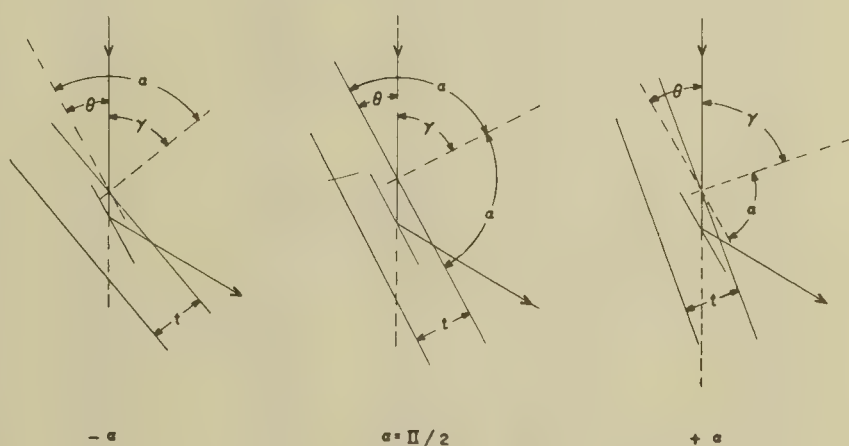


Fig. 5.3.8(3)

TABLE 5.3.6B
Absorption Correction Factors A* for Successive Values of θ
Spheres of Radius R

μR	0°	5°	10°	15°	20°	25°	30°	35°	40°	45°
0	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
0.1	1.16	1.16	1.16	1.16	1.16	1.16	1.16	1.16	1.16	1.16
0.2	1.35	1.35	1.35	1.34	1.34	1.34	1.34	1.34	1.34	1.34
0.3	1.56	1.56	1.56	1.55	1.55	1.55	1.55	1.54	1.54	1.53
0.4	1.80	1.80	1.80	1.79	1.79	1.78	1.78	1.77	1.76	1.75
0.5	2.08	2.07	2.07	2.06	2.06	2.05	2.03	2.02	2.01	1.99
0.6	2.39	2.39	2.38	2.37	2.36	2.34	2.32	2.30	2.27	2.25
0.7	2.75	2.74	2.73	2.72	2.70	2.67	2.64	2.60	2.57	2.53
0.8	3.15	3.15	3.13	3.11	3.07	3.03	2.99	2.94	2.89	2.83
0.9	3.61	3.60	3.58	3.54	3.50	3.44	3.37	3.30	3.23	3.16
1.0	4.12	4.11	4.08	4.03	3.96	3.88	3.79	3.70	3.60	3.50
1.1	4.70	4.69	4.64	4.57	4.48	4.37	4.25	4.12	3.99	3.87
1.2	5.35	5.33	5.27	5.17	5.05	4.90	4.74	4.57	4.41	4.25
1.3	6.08	6.05	5.97	5.84	5.67	5.47	5.27	5.06	4.85	4.66
1.4	6.90	6.86	6.75	6.57	6.35	6.10	5.83	5.57	5.32	5.08
1.5	7.80	7.75	7.60	7.38	7.09	6.77	6.44	6.11	5.81	5.52
1.6	8.81	8.74	8.55	8.25	7.89	7.49	7.08	6.69	6.32	5.98
1.7	9.92	9.83	9.59	9.21	8.76	8.26	7.76	7.29	6.85	6.45
1.8	11.2	11.0	10.7	10.3	9.69	9.08	8.48	7.92	7.40	6.94
1.9	12.5	12.4	12.0	11.4	10.7	9.95	9.24	8.58	7.98	7.44
2.0	14.0	13.8	13.3	12.6	11.8	10.9	10.0	9.26	8.57	7.96
2.1	15.6	15.4	14.8	13.9	12.9	11.8	10.9	9.97	9.18	8.49
2.2	17.4	17.1	16.4	15.3	14.1	12.9	11.7	10.7	9.80	9.03
2.3	19.4	19.0	18.1	16.8	15.3	13.9	12.6	11.4	10.4	9.57
2.4	21.5	21.0	19.9	18.4	16.7	15.0	13.5	12.2	11.1	10.1
2.5	23.8	23.3	21.9	20.0	18.1	16.2	14.5	13.0	11.7	10.7
2.6	26.3	25.6	24.0	21.8	19.5	17.3	15.4	13.8	12.4	11.3
2.7	29.0	28.2	26.2	23.7	21.0	18.6	16.4	14.6	13.1	11.8
2.8	31.9	30.9	28.6	25.6	22.6	19.8	17.4	15.4	13.8	12.4
2.9	35.0	33.9	31.2	27.7	24.2	21.1	18.5	16.3	14.5	13.0
3.0	38.4	37.0	33.9	29.9	25.9	22.4	19.5	17.1	15.2	13.6
3.1	42.0	40.4	36.7	32.1	27.7	23.8	20.6	18.0	15.9	14.2
3.2	45.8	43.9	39.7	34.4	29.5	25.2	21.7	18.9	16.6	14.8
3.3	49.9	47.7	42.8	36.8	31.3	26.6	22.8	19.8	17.4	15.4
3.4	54.3	51.7	46.0	39.3	33.2	28.1	23.9	20.7	18.1	16.1
3.5	58.9	56.0	49.5	41.9	35.2	29.5	25.1	21.6	18.9	16.7
3.6	63.8	60.4	53.0	44.6	37.1	31.0	26.2	22.5	19.6	17.3
3.7	69.0	65.1	56.8	47.3	39.2	32.6	27.4	23.4	20.4	17.9
3.8	74.6	70.1	60.6	50.2	41.2	34.1	28.6	24.4	21.1	18.6
3.9	80.4	75.3	64.6	53.1	43.3	35.7	29.3	25.3	21.9	19.2
4.0	86.5	80.7	68.8	56.0	45.5	37.2	31.0	26.3	22.7	19.8
4.1	93.0	86.4	73.1	59.1	47.6	38.8	32.2	27.2	23.4	20.5
4.2	99.8	92.4	77.5	62.2	49.9	40.5	33.4	28.2	24.2	21.1
4.3	107	98.6	82.1	65.3	52.1	42.1	34.7	29.2	25.0	21.8
4.4	114	105	86.8	68.6	54.4	43.7	35.9	30.1	25.8	22.4
4.5	122	112	91.7	71.9	56.7	45.4	37.2	31.1	26.6	23.1
4.6	130	119	96.7	75.2	59.0	47.1	38.4	32.1	27.4	23.7
4.7	139	126	102	78.6	61.3	48.8	39.7	33.1	28.1	24.4
4.8	148	134	107	82.1	63.7	50.5	41.0	34.1	28.9	25.0
4.9	157	141	112	85.6	66.1	52.2	42.2	35.1	29.7	25.7

TABLE 5.3.6B (*continued*)
Absorption Correction Factors A* for Successive Values of θ
Spheres of Radius R

50°	55°	60°	65°	70°	75°	80°	85°	90°	μR
1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	0
1.16	1.16	1.16	1.16	1.16	1.16	1.16	1.16	1.16	0.1
1.33	1.33	1.33	1.33	1.33	1.33	1.33	1.33	1.33	0.2
1.53	1.53	1.52	1.52	1.51	1.51	1.51	1.51	1.51	0.3
1.74	1.73	1.73	1.72	1.71	1.70	1.70	1.70	1.70	0.4
1.97	1.96	1.94	1.93	1.92	1.91	1.90	1.90	1.90	0.5
2.23	2.20	2.18	2.16	2.14	2.13	2.11	2.11	2.11	0.6
2.50	2.46	2.43	2.40	2.37	2.35	2.33	2.32	2.32	0.7
2.78	2.73	2.69	2.65	2.61	2.58	2.56	2.55	2.55	0.8
3.09	3.02	2.96	2.91	2.86	2.82	2.80	2.78	2.77	0.9
3.41	3.33	3.25	3.18	3.12	3.07	3.04	3.02	3.01	1.0
3.75	3.64	3.55	3.46	3.39	3.33	3.28	3.26	3.25	1.1
4.11	3.97	3.85	3.75	3.66	3.59	3.54	3.50	3.49	1.2
4.48	4.32	4.17	4.04	3.94	3.85	3.79	3.75	3.73	1.3
4.86	4.67	4.49	4.34	4.22	4.12	4.05	4.00	3.98	1.4
5.26	5.03	4.83	4.65	4.51	4.39	4.31	4.26	4.23	1.5
5.67	5.40	5.17	4.97	4.80	4.67	4.57	4.51	4.48	1.6
6.10	5.78	5.51	5.28	5.09	4.94	4.83	4.77	4.74	1.7
6.53	6.17	5.87	5.60	5.39	5.22	5.10	5.02	4.99	1.8
6.97	6.57	6.22	5.93	5.69	5.50	5.37	5.28	5.25	1.9
7.43	6.97	6.59	6.26	5.99	5.78	5.63	5.54	5.50	2.0
7.89	7.38	6.95	6.59	6.30	6.07	5.90	5.80	5.76	2.1
8.36	7.80	7.33	6.93	6.61	6.36	6.17	6.06	6.02	2.2
8.84	8.22	7.70	7.27	6.92	6.64	6.45	6.32	6.28	2.3
9.32	8.65	8.08	7.61	7.23	6.93	6.72	6.59	6.54	2.4
9.81	9.07	8.46	7.95	7.54	7.23	6.99	6.85	6.80	2.5
10.3	9.51	8.85	8.30	7.86	7.52	7.27	7.12	7.06	2.6
10.8	9.94	9.23	8.64	8.17	7.81	7.54	7.38	7.33	2.7
11.3	10.4	9.62	8.99	8.49	8.10	7.82	7.65	7.59	2.8
11.8	10.8	10.0	9.34	8.81	8.40	8.10	7.92	7.85	2.9
12.3	11.3	10.4	9.70	9.13	8.70	8.38	8.18	8.11	3.0
12.8	11.7	10.8	10.0	9.45	8.99	8.66	8.45	8.38	3.1
13.4	12.2	11.2	10.4	9.77	9.29	8.94	8.72	8.64	3.2
13.9	12.6	11.6	10.8	10.1	9.59	9.21	8.99	8.90	3.3
14.4	13.1	12.0	11.1	10.4	9.88	9.49	9.25	9.17	3.4
14.9	13.5	12.4	11.5	10.7	10.2	9.77	9.52	9.43	3.5
15.5	14.0	12.8	11.8	11.1	10.5	10.1	9.79	9.69	3.6
16.0	14.5	13.2	12.2	11.4	10.8	10.3	10.1	9.96	3.7
16.5	14.9	13.6	12.6	11.7	11.1	10.6	10.3	10.2	3.8
17.1	15.4	14.0	12.9	12.0	11.4	10.9	10.6	10.5	3.9
17.6	15.8	14.4	13.3	12.4	11.7	11.2	10.9	10.8	4.0
18.2	16.3	14.8	13.6	12.7	12.0	11.5	11.1	11.0	4.1
18.7	16.8	15.2	14.0	13.0	12.3	11.7	11.4	11.3	4.2
19.3	17.2	15.7	14.4	13.4	12.6	12.0	11.7	11.5	4.3
19.8	17.7	16.1	14.7	13.7	12.9	12.3	11.9	11.8	4.4
20.3	18.2	16.5	15.1	14.0	13.2	12.6	12.2	12.1	4.5
20.9	18.7	16.9	15.5	14.3	13.5	12.9	12.5	12.3	4.6
21.4	19.1	17.3	15.8	14.7	13.8	13.2	12.8	12.6	4.7
22.0	19.6	17.7	16.2	15.0	14.1	13.4	13.0	12.9	4.8
22.6	20.1	18.1	16.6	15.3	14.4	13.7	13.3	13.1	4.9

TABLE 5.3.6B (continued)
Absorption Correction Factors A* for Successive Values of θ
Spheres of Radius R

μR	0°	5°	10°	15°	20°	25°	30°	35°	40°	45°
5.0	167	150	118	89.1	68.5	53.9	43.5	36.1	30.5	26.4
5.1	177	158	124	92.7	71.0	55.6	44.8	37.1	31.3	27.0
5.2	188	167	129	96.4	73.4	57.4	46.1	38.1	32.2	27.7
5.3	199	176	135	100	75.9	59.2	47.4	39.1	33.0	28.3
5.4	210	185	141	104	78.4	60.9	48.8	40.1	33.8	29.0
5.5	222	194	147	108	80.9	62.7	50.1	41.1	34.6	29.7
5.6	234	204	153	111	83.5	64.5	51.4	42.2	35.4	30.3
5.7	247	214	160	115	86.0	66.3	52.7	43.2	36.2	31.0
5.8	260	224	166	119	88.6	68.1	54.1	44.2	37.0	31.7
5.9	274	235	173	123	91.2	69.9	55.4	45.2	37.9	32.3
6.0	288	246	179	127	93.8	71.7	56.8	46.3	38.7	33.0
6.1	303	257	186	131	96.4	73.6	58.1	47.3	39.5	33.7
6.2	318	269	193	135	99.1	75.4	59.5	48.4	40.3	34.4
6.3	334	280	200	139	102	77.2	60.8	49.4	41.2	35.0
6.4	350	293	207	143	104	79.1	62.2	50.4	42.0	35.7
6.5	366	305	214	148	107	81.0	63.5	51.5	42.8	36.4
6.6	383	318	221	152	110	82.8	64.9	52.5	43.6	37.1
6.7	401	331	229	156	112	84.7	66.3	53.6	44.5	37.8
6.8	419	344	236	160	115	86.6	67.7	54.6	45.3	38.4
6.9	438	357	244	165	118	88.5	69.0	55.7	46.1	39.1
7.0	457	371	251	169	121	90.4	70.4	56.7	47.0	39.8
7.1	477	385	259	173	123	92.2	71.8	57.8	47.8	40.5
7.2	498	400	267	177	126	94.1	73.2	58.9	48.7	41.2
7.3	519	415	275	182	129	96.0	74.6	59.9	49.5	41.8
7.4	540	430	283	186	132	98.0	76.0	61.0	50.3	42.5
7.5	563	445	291	191	135	99.9	77.4	62.0	51.2	43.2
7.6	585	460	299	195	137	102	78.8	63.1	52.0	43.9
7.7	609	476	307	200	140	104	80.2	64.2	52.8	44.6
7.8	633	493	315	204	143	106	81.6	65.2	53.7	45.3
7.9	657	509	324	209	146	108	83.0	66.3	54.5	45.9
8.0	683	526	332	213	149	110	84.4	67.4	55.4	46.6
8.1	709	543	341	218	152	111	85.8	68.4	56.2	47.3
8.2	735	560	349	222	154	113	87.2	69.5	57.1	48.0
8.3	762	578	358	227	157	115	88.6	70.6	57.9	48.7
8.4	790	596	367	232	160	117	90.1	71.7	58.8	49.4
8.5	819	614	375	236	163	119	91.5	72.7	59.6	50.1
8.6	848	632	384	241	166	121	92.9	73.8	60.4	50.7
8.7	878	651	393	246	169	123	94.3	74.9	61.3	51.4
8.8	909	670	402	250	172	125	95.8	76.0	62.1	52.1
8.9	940	690	411	255	175	127	97.2	77.1	63.0	52.8
9.0	972	709	420	260	178	129	98.6	78.2	63.9	53.5
9.1	1005	729	429	264	180	131	100	79.3	64.7	54.2
9.2	1038	749	439	269	183	133	101	80.4	65.6	54.9
9.3	1072	770	448	274	186	135	103	81.5	66.4	55.6
9.4	1107	791	457	279	189	137	104	82.6	67.3	56.3
9.5	1143	812	467	284	192	139	106	83.7	68.2	57.0
9.6	1180	833	476	288	195	141	107	84.8	69.1	57.7
9.7	1217	855	485	293	198	143	109	85.9	69.9	58.4
9.8	1255	877	495	298	201	145	110	87.0	70.8	59.1
9.9	1294	899	505	303	204	147	112	88.2	71.7	59.8
10.0	1333	921	514	308	207	149	113	89.3	72.6	60.5

TABLE 5.3.6B (*continued*)
Absorption Correction Factors A* for Successive Values of θ
Spheres of Radius R

50°	55°	60°	65°	70°	75°	80°	85°	90°	μR
23.1	20.6	18.5	16.9	15.7	14.7	14.0	13.6	13.4	5.0
23.7	21.0	19.0	17.3	16.0	15.0	14.3	13.8	13.7	5.1
24.2	21.5	19.4	17.7	16.3	15.3	14.6	14.1	13.9	5.2
24.8	22.0	19.8	18.0	16.7	15.6	14.9	14.4	14.2	5.3
25.3	22.5	20.2	18.4	17.0	15.9	15.1	14.6	14.5	5.4
25.9	22.9	20.6	18.8	17.3	16.2	15.4	14.9	14.7	5.5
26.4	23.4	21.0	19.1	17.7	16.5	15.7	15.2	15.0	5.6
27.0	23.9	21.5	19.5	18.0	16.8	16.0	15.5	15.3	5.7
27.6	24.4	21.9	19.9	18.3	17.2	16.3	15.7	15.5	5.8
28.1	24.9	22.3	20.3	18.7	17.5	16.6	16.0	15.8	5.9
28.7	25.3	22.7	20.6	19.0	17.8	16.8	16.3	16.1	6.0
29.3	25.8	23.1	21.0	19.3	18.1	17.1	16.5	16.3	6.1
29.8	26.3	23.6	21.4	19.7	18.4	17.4	16.8	16.6	6.2
30.4	26.8	24.0	21.7	20.0	18.7	17.7	17.1	16.9	6.3
31.0	27.3	24.4	22.1	20.3	19.0	18.0	17.4	17.1	6.4
31.5	27.8	24.8	22.5	20.7	19.3	18.3	17.6	17.4	6.5
32.1	28.2	25.2	22.9	21.0	19.6	18.5	17.9	17.7	6.6
32.7	28.7	25.7	23.2	21.3	19.9	18.8	18.2	17.9	6.7
33.2	29.2	26.1	23.6	21.7	20.2	19.1	18.4	18.2	6.8
33.8	29.7	26.5	24.0	22.0	20.5	19.4	18.7	18.4	6.9
34.4	30.2	26.9	24.3	22.3	20.8	19.7	19.0	18.7	7.0
34.9	30.7	27.3	24.7	22.7	21.1	20.0	19.3	19.0	7.1
35.5	31.1	27.8	25.1	23.0	21.4	20.3	19.5	19.2	7.2
36.1	31.6	28.2	25.5	23.4	21.7	20.5	19.8	19.5	7.3
36.6	32.1	28.6	25.8	23.7	22.1	20.8	20.1	19.8	7.4
37.2	32.6	29.0	26.2	24.0	22.4	21.1	20.3	20.0	7.5
37.8	33.1	29.4	26.6	24.4	22.7	21.4	20.6	20.3	7.6
38.4	33.6	29.9	27.0	24.7	23.0	21.7	20.9	20.6	7.7
38.9	34.1	30.3	27.3	25.0	23.3	22.0	21.2	20.8	7.8
39.5	34.6	30.7	27.7	25.4	23.6	22.3	21.4	21.1	7.9
40.1	35.0	31.1	28.1	25.7	23.9	22.5	21.7	21.4	8.0
40.6	35.5	31.6	28.5	26.0	24.2	22.8	22.0	21.6	8.1
41.2	36.0	32.0	28.8	26.4	24.5	23.1	22.2	21.9	8.2
41.8	36.5	32.4	29.2	26.7	24.8	23.4	22.5	22.2	8.3
42.4	37.0	32.9	29.6	27.1	25.1	23.7	22.8	22.4	8.4
42.9	37.5	33.3	30.0	27.4	25.4	24.0	23.1	22.7	8.5
43.5	38.0	33.7	30.3	27.7	25.7	24.3	23.3	23.0	8.6
44.1	38.5	34.1	30.7	28.1	26.1	24.5	23.6	23.2	8.7
44.7	39.0	34.6	31.1	28.4	26.4	24.8	23.9	23.5	8.8
45.2	39.5	35.0	31.5	28.7	26.7	25.1	24.2	23.8	8.9
45.8	39.9	35.4	31.8	29.1	27.0	25.4	24.4	24.0	9.0
46.4	40.4	35.8	32.2	29.4	27.3	25.7	24.7	24.3	9.1
46.9	40.9	36.2	32.6	29.7	27.6	26.0	25.0	24.6	9.2
47.5	41.3	36.6	32.9	30.1	27.9	26.3	25.2	24.8	9.3
48.0	41.8	37.0	33.3	30.4	28.2	26.5	25.5	25.1	9.4
48.6	42.2	37.4	33.6	30.7	28.5	26.8	25.8	25.4	9.5
49.1	42.7	37.7	33.9	31.0	28.8	27.1	26.1	25.6	9.6
49.6	43.1	38.1	34.3	31.4	29.1	27.4	26.3	25.9	9.7
50.2	43.5	38.4	34.6	31.7	29.5	27.7	26.6	26.2	9.8
50.7	43.9	38.7	34.9	32.0	29.8	28.0	26.9	26.4	9.9
51.2	44.2	39.0	35.2	32.3	30.1	28.3	27.2	26.7	10.0

5.3. ABSORPTION CORRECTIONS

(Continued from page 301)

expressions are also given here, the transmission case being that described by Decker, Asp and Harker [26], and the reflection case the one called Case III by Schwartz [36]. The transmission and reflection counter techniques may be used together on the same sample to produce the complete pole figure.

The symbols indicated in Figures 5.3.8(1) (2) and (3) are as follows:

γ = acute angle between the sheet normal and the incident beam.

ϕ = azimuthal angle around the diffraction ring; this ring intersects the plane containing the incident beam and the normal to the surface of the specimen at two points. For the transmission case, ϕ is taken as zero at the intersection point which is nearest to the sample when the reflecting planes are normal to the surface of the sheet. For the reflection case, $\phi=0$ at the intersection point contained in the reflection region.

t = thickness of the sheet.

x = distance traversed by beam before diffraction occurs, projected on to t .

α = acute angle between the sheet normal and the diffracting plane. The sign of α is defined as shown in Figs. 5.3.8(2) and 5.3.8(3).

K = a constant which includes factors representing the intensity of the incident beam and the structure factor for the reflection. K will be cancelled when taking the ratio of two intensities for the same sample, reflection and radiation.

In the following treatment absolute values of the angles have been used; their directions are taken care of in the signs in the algebraic expressions.

5.3.8.1. TRANSMISSION CASE

(a) General Expression (see Fig. 5.3.8(1))

$$I_{\phi,\gamma} = KA \int_0^t e^{Bx} \frac{dx}{\cos \gamma} = K \frac{A(e^{Bt}-1)}{B \cos \gamma} \quad \dots (17)$$

where $A = e^{-\mu t C}$

$$B = -\mu \left(\frac{1}{\cos \gamma} - C \right)$$

$$C = \frac{1}{\cos \gamma \cos 2\theta - \sin \gamma \sin 2\theta \cos \phi}$$

(b) Special Case for Counter Technique (see Fig. 5.3.8(2))

$$\gamma = \theta \pm \alpha; \quad \phi = \pi$$

$$I_{\pm\alpha} = K \frac{A(e^{Bt}-1)}{B \cos (\theta \pm \alpha)}$$

where $A = e^{-\mu t C}$

$$B = -\mu \left(\frac{1}{\cos (\theta \pm \alpha)} - C \right)$$

$$C = \frac{1}{\cos (\theta \mp \alpha)}$$

$$I_{\alpha=0} = K \frac{t}{\cos \theta} e^{-\mu t / \cos \theta}$$

$$\frac{I_{\alpha=0}}{I_{\pm\alpha}} = W_{\theta} e^{-W_{\theta}} \left[\frac{\frac{W_{\theta \mp \alpha} - 1}{W_{\theta \pm \alpha}}}{e^{-W_{\theta \pm \alpha}} - e^{-W_{\theta \mp \alpha}}} \right] \quad \dots (18)$$

where W is of the form $W_{\Sigma} = \mu t / \cos \Sigma$.

In practice it is better to use α in the negative region only, since unknown factors which seem to be dependent on the diffracting volume affect the transmitted intensity. The change in diffracting volume is small in the negative region of α , but increases quite rapidly as α increases in the positive region.

A table of intensity correction factors for this special transmission case using counter technique was prepared by Beatty. This table, expanded to include smaller intervals in the value of $e^{-\mu t}$, is reproduced as Table 5.3.8. The quantity listed is $100 I_{\alpha=0} / I_{-\alpha}$ of equation 5.3.8 (18) for specified values of α , 2θ and $e^{-\mu t}$.

5.3.8.2. REFLECTION CASE

(a) General Expression

$$I_{\phi,\gamma} = K \int_0^t e^{Bx} \frac{dx}{\cos \gamma} = K \frac{(e^{Bt}-1)}{B \cos \gamma} \quad \dots (19)$$

$$\text{where } B = -\mu \left(\frac{1}{\cos \gamma} - \frac{1}{\cos \gamma \cos 2\theta - \sin \gamma \sin 2\theta \cos \phi} \right)$$

(b) Special Case for Counter Technique (see Fig. 5.3.8(3))

$$+\alpha \text{ region: } \gamma = \pi - (\alpha + \theta); \quad \phi = 0$$

$$-\alpha \text{ region: } \gamma = \alpha - \theta; \quad \phi = 0$$

$$I_{\pm\alpha} = K \frac{(e^{Bt}-1)}{\mp B \cos (\theta \pm \alpha)}$$

$$\text{where } B = -\mu \left(\frac{1}{\cos (\theta - \alpha)} - \frac{1}{\cos (\theta + \alpha)} \right)$$

$$\frac{I_{\alpha=0}}{I_{\pm\alpha}} = W_{\theta} e^{-W_{\theta}} \left[\frac{\frac{W_{\theta \mp \alpha} - 1}{W_{\theta \pm \alpha}}}{e^{(W_{\theta + \alpha} - W_{\theta - \alpha})} - 1} \right] \quad \dots (20)$$

where W is of the form $W_{\Sigma} = \mu t / \cos \Sigma$ and the expression for $I_{\alpha=0}$ is taken from the above treatment for the transmission case.

In practice it is better to use α in the positive region only, since the correction factor changes quite rapidly in the negative region.

5.3. ABSORPTION CORRECTIONS

TABLE 5.3.8

(A recalculation and extension of a table prepared by S. V. D. Beatty, and used by permission of the Westinghouse Research Laboratories)

Intensity Correction Factors for X-ray Spectrometer

Transmission Pole Figure Determinations $100 \frac{I_{\alpha=0}}{I_{-\alpha}}$ of equation 5.3.8(18)

$e^{-\mu t}$	$2\theta = 10^\circ$	20°	30°	40°	50°	60°	70°	80°
$\alpha = 5^\circ$								
0.01	102	103	104	105	106	107	108	109
0.02	102	103	104	105	106	107	108	109
0.03	102	103	103	104	105	107	108	109
0.04	102	102	103	104	105	107	108	109
0.05	102	102	103	104	105	106	108	109
0.06	101	102	103	104	105	106	108	109
0.07	101	102	103	104	105	106	108	109
0.08	101	102	103	104	105	106	108	109
0.09	101	102	103	104	105	106	108	109
0.10	101	102	103	104	105	106	107	109
0.20	101	102	103	104	105	106	107	109
0.30	101	102	102	103	104	105	107	108
0.40	101	102	102	103	104	105	107	108
0.50	101	101	102	103	104	105	106	108
0.60	101	101	102	103	104	105	106	108
0.70	101	101	102	103	104	105	106	107
0.80	100	101	102	103	104	105	106	107
0.90	100	101	102	103	104	105	106	107
$\alpha = 10^\circ$								
0.01	107	109	111	113	116	118	121	124
0.02	106	108	110	112	115	118	121	124
0.03	106	107	109	112	114	117	120	124
0.04	105	107	109	111	114	117	120	124
0.05	105	107	109	111	113	116	120	124
0.06	104	106	108	110	113	116	119	123
0.07	104	106	108	110	113	116	119	123
0.08	104	106	108	110	112	115	119	123
0.09	104	106	108	110	112	115	118	123
0.10	104	105	107	109	112	115	118	122
0.20	103	104	106	108	110	113	116	120
0.30	102	104	105	107	110	112	115	119
0.40	101	103	105	107	109	111	114	118
0.50	101	103	104	106	108	111	113	117
0.60	101	102	104	106	108	110	113	116
0.70	101	102	104	106	107	110	112	115
0.80	100	102	104	105	107	109	112	114
0.90	100	102	103	105	107	109	111	114

5.3. ABSORPTION CORRECTIONS

TABLE 5.3.8 (continued)

Intensity Correction Factors for X-ray Spectrometer

Transmission Pole Figure Determinations $100 \frac{I_{\alpha=0}}{I_{-\alpha}}$ of equation 5.3.8(18)

$e^{-\mu t}$	$2\theta = 10^\circ$	20°	30°	40°	50°	60°	70°	80°
$\alpha = 15^\circ$								
0.01	116	120	123	127	131	136	141	145
0.02	114	117	120	124	129	134	140	146
0.03	112	115	119	123	127	133	139	146
0.04	111	114	117	121	126	131	138	146
0.05	110	113	116	120	125	130	137	145
0.06	109	112	116	120	124	130	136	145
0.07	109	112	115	119	123	129	136	144
0.08	108	111	114	118	123	128	135	143
0.09	108	111	114	118	122	128	134	143
0.10	107	110	113	117	122	127	134	142
0.20	105	107	110	114	118	123	129	137
0.30	103	106	109	112	116	120	126	133
0.40	102	105	108	111	114	118	123	130
0.50	101	104	107	110	113	117	121	127
0.60	101	103	106	109	112	115	120	125
0.70	100	103	105	108	111	114	118	123
0.80	100	102	104	107	110	113	117	121
0.90	99	102	104	107	109	112	116	120
$\alpha = 20^\circ$								
0.01	131	135	141	148	155	162	170	176
0.02	125	130	135	142	150	159	169	179
0.03	122	126	132	138	146	156	167	180
0.04	119	124	130	136	144	153	165	179
0.05	118	122	128	134	142	151	163	178
0.06	116	121	126	132	140	150	161	177
0.07	115	120	125	131	139	148	160	175
0.08	114	119	124	130	137	147	159	174
0.09	113	118	123	129	136	145	157	173
0.10	113	117	122	128	135	144	156	172
0.20	108	112	116	121	128	136	147	161
0.30	105	109	113	118	124	131	140	153
0.40	103	107	110	115	120	127	135	146
0.50	101	105	109	113	118	124	131	141
0.60	100	104	107	111	116	121	128	136
0.70	99	103	106	110	114	119	125	132
0.80	98	102	105	109	112	117	122	129
0.90	98	101	104	107	111	115	120	126

5.3. ABSORPTION CORRECTIONS

TABLE 5.3.8 (continued)

Intensity Correction Factors for X-ray Spectrometer

Transmission Pole Figure Determinations $100 \frac{I_{\alpha=0}}{I_{-\alpha}}$ of equation 5.3.8(18)

$e^{-\mu t}$	$2\theta = 10^\circ$	20°	30°	40°	50°	60°	70°	80°
$\alpha = 25^\circ$								
0.01	152	160	169	179	190	202	214	223
0.02	142	149	158	168	181	195	212	229
0.03	136	143	152	162	174	190	209	230
0.04	132	139	147	157	170	186	205	230
0.05	129	136	144	154	166	182	202	228
0.06	127	133	141	151	163	179	199	226
0.07	125	131	139	148	160	176	197	224
0.08	123	129	137	146	158	174	194	222
0.09	121	128	135	144	156	171	192	220
0.10	120	126	134	143	154	169	190	218
0.20	112	117	124	131	141	154	172	198
0.30	107	112	118	125	134	145	160	183
0.40	104	109	114	120	128	138	151	170
0.50	101	106	111	117	124	132	144	160
0.60	100	104	109	114	120	128	138	151
0.70	98	102	107	112	117	124	132	144
0.80	97	101	105	109	115	121	128	137
0.90	95	99	103	108	112	118	124	131
$\alpha = 30^\circ$								
0.01	186	198	211	227	245	263	281	297
0.02	167	178	192	208	228	252	279	309
0.03	157	168	181	197	217	243	274	312
0.04	151	161	173	189	209	235	269	311
0.05	145	155	167	183	203	229	264	309
0.06	141	151	163	178	198	224	259	307
0.07	138	147	159	174	193	219	254	304
0.08	135	144	155	170	189	214	250	300
0.09	133	141	152	167	185	211	246	297
0.10	131	139	150	164	182	207	242	293
0.20	117	125	134	145	160	181	212	260
0.30	110	117	125	134	147	165	191	232
0.40	105	111	118	127	138	153	175	209
0.50	101	107	114	121	131	144	162	190
0.60	99	104	110	117	125	136	151	174
0.70	96	101	107	113	121	130	142	160
0.80	94	99	104	110	117	124	134	148
0.90	93	97	102	107	113	120	128	138

5.3. ABSORPTION CORRECTIONS

TABLE 5.3.8 (continued)

Intensity Correction Factors for X-ray Spectrometer

Transmission Pole Figure Determinations $100 \frac{I_{\alpha=0}}{I_{-\alpha}}$ of equation 5.3.8(18)

$e^{-\mu t}$	$2\theta = 10^\circ$	20°	30°	40°	50°	60°	70°	80°
$\alpha = 35^\circ$								
0.01	242	260	281	305	332	361	391	427
0.02	208	224	245	271	303	341	388	447
0.03	190	206	226	252	285	327	380	453
0.04	178	193	213	238	271	314	372	454
0.05	170	184	203	227	260	304	364	451
0.06	163	177	195	219	251	295	357	448
0.07	158	171	188	211	243	287	349	444
0.08	153	166	183	205	236	279	342	439
0.09	149	162	178	200	230	273	336	434
0.10	146	158	174	195	224	267	329	428
0.20	125	135	147	164	188	223	277	372
0.30	114	123	133	148	167	195	240	322
0.40	107	115	124	136	152	175	212	279
0.50	102	109	117	127	141	160	190	243
0.60	98	104	112	121	132	148	171	212
0.70	94	100	107	115	125	138	156	186
0.80	91	97	103	110	119	129	143	164
0.90	89	94	100	106	113	122	132	146
$\alpha = 40^\circ$								
0.01	337	366	399	437	478	526	590	701
0.02	274	300	334	376	427	493	582	736
0.03	242	267	299	341	395	468	570	746
0.04	222	245	276	317	372	447	557	748
0.05	208	229	259	298	353	430	544	745
0.06	196	217	245	284	337	415	532	740
0.07	187	207	234	271	324	401	520	733
0.08	180	199	225	261	312	389	508	725
0.09	173	192	217	252	302	377	497	717
0.10	168	186	210	244	293	367	487	708
0.20	136	149	168	194	232	293	399	612
0.30	120	131	146	167	197	246	333	520
0.40	109	119	132	149	173	212	282	436
0.50	102	111	122	136	156	186	241	362
0.60	96	104	114	126	142	166	207	298
0.70	92	99	108	118	131	149	180	243
0.80	88	95	102	111	121	135	157	198
0.90	85	91	98	105	113	124	138	161

5.3. ABSORPTION CORRECTIONS

TABLE 5.3.8 (continued)

Intensity Correction Factors for X-ray Spectrometer

Transmission Pole Figure Determinations $100 \frac{I_{\alpha=0}}{I_{-\alpha}}$ of equation 5.3.8(18)

$e^{-\mu t}$	$2\theta = 10^\circ$	20°	30°	40°	50°	60°	70°	80°
$\alpha = 45^\circ$								
0.01	520	566	618	674	741	838	1020	1564
0.02	392	436	491	559	647	774	999	1637
0.03	333	373	426	496	590	728	973	1658
0.04	296	333	384	453	548	691	948	1660
0.05	270	305	353	420	516	661	923	1653
0.06	250	283	329	394	488	634	900	1640
0.07	235	266	310	372	465	611	878	1624
0.08	222	252	294	354	445	590	857	1605
0.09	212	240	280	338	427	570	837	1586
0.10	203	230	268	325	411	553	818	1566
0.20	152	171	199	240	307	423	660	1349
0.30	128	144	165	197	248	340	538	1140
0.40	113	126	144	169	208	280	439	946
0.50	103	114	129	149	180	234	356	766
0.60	96	105	117	134	157	198	288	599
0.70	90	98	108	121	140	170	232	447
0.80	85	92	101	112	126	146	186	314
0.90	80	87	95	103	114	127	149	208
$\alpha = 50^\circ$								
0.01	913	986	1056	1140	1271	1546	2412	
0.02	629	704	794	910	1080	1398	2331	
0.03	505	574	665	787	968	1300	2252	
0.04	431	495	583	705	889	1225	2181	
0.05	382	441	524	644	827	1164	2115	
0.06	345	400	480	596	777	1111	2055	
0.07	317	369	444	557	735	1065	1999	
0.08	295	343	415	524	698	1024	1946	
0.09	276	322	390	495	666	986	1896	
0.10	260	304	369	470	637	952	1849	
0.20	177	206	250	322	450	709	1470	
0.30	141	163	195	248	345	552	1185	
0.40	120	137	162	202	275	436	952	
0.50	106	120	140	170	224	345	751	
0.60	95	107	123	147	187	273	575	
0.70	87	97	110	128	157	216	421	
0.80	81	90	100	114	134	172	292	
0.90	75	83	92	102	115	136	191	

5.3. ABSORPTION CORRECTIONS

TABLE 5.3.8 (continued)

Intensity Correction Factors for X-ray Spectrometer

Transmission Pole Figure Determinations $100 \frac{I_{\alpha=0}}{I_{-\alpha}}$ of equation 5.3.8(18)

$e^{-\mu t}$	$2\theta = 10^\circ$	20°	30°	40°	50°	60°
$\alpha = 55^\circ$						
0.01	1926	2000	2052	2182	2566	3946
0.02	1179	1304	1447	1663	2104	3473
0.03	882	1006	1165	1399	1847	3179
0.04	717	833	991	1228	1670	2961
0.05	610	718	871	1104	1537	2788
0.06	534	634	780	1008	1430	2643
0.07	477	570	710	930	1341	2518
0.08	433	520	652	865	1265	2408
0.09	397	478	605	810	1199	2309
0.10	367	444	564	763	1140	2220
0.20	220	267	345	484	769	1608
0.30	162	195	249	349	566	1228
0.40	130	155	195	267	429	949
0.50	110	129	159	212	330	726
0.60	96	111	134	172	255	543
0.70	85	98	115	142	198	390
0.80	77	87	100	119	155	266
0.90	70	79	89	102	121	171
$\alpha = 60^\circ$						
0.01	5278	4960	4729	5078	7328	
0.02	2775	2906	3089	3649	5738	
0.03	1895	2100	2375	2966	4905	
0.04	1442	1656	1955	2540	4353	
0.05	1165	1373	1673	2240	3946	
0.06	978	1174	1467	2013	3628	
0.07	842	1026	1308	1834	3367	
0.08	740	912	1182	1686	3149	
0.09	660	820	1078	1563	2960	
0.10	595	745	992	1457	2796	
0.20	300	386	542	862	1802	
0.30	199	255	360	587	1285	
0.40	149	188	260	422	946	
0.50	118	147	198	312	697	
0.60	98	120	156	234	505	
0.70	84	100	126	177	354	
0.80	73	85	103	136	236	
0.90	64	74	86	105	150	

5.4. Mosaic Theory

Equations 5.5 (1)–(11) have been derived on the assumption that the intensity of the X-ray beam passing through a crystal is not affected by the process of diffraction. This is true only if the crystal is composed of small parts that scatter quite independently, a condition which is completely disobeyed by a perfect crystal. (“Real” crystals, however, do obey the condition approximately; they are composed of small blocks (mosaic blocks) which are in sufficient disregistry to scatter independently.) Few crystals, however, are sufficiently imperfect for equations 5.5 (1)–(11) to apply to all the X-ray reflections; on the other hand, none is so perfect that equations based on crystal perfection apply.

The problem was first studied by Darwin [44], who showed that a perfect crystal should obey the relation

$$\int R(\theta) d\theta = \frac{8}{3\pi} N \lambda^2 |F| \frac{e^2}{mc^2} \frac{1 + |\cos 2\theta|}{2 \sin 2\theta} \dots (1)$$

The integrated reflection is thus proportional to $|F|$ and not to $|F|^2$. Integrated reflections for perfect crystals are much weaker than for imperfect crystals.

The difference between the formulae for the two types of crystal arises because of the interaction between the scattered radiation and the incident radiation. It can be shown by the ordinary Fresnel construction that the rays scattered by a complete plane of atoms are such that they have a phase difference of $\pi/2$ with respect to the rays scattered in the same direction by a single point. Reflected rays must be incident upon the reverse side of the reflecting planes at the correct Bragg angle for reflection, and the twice-reflected rays will then have a direction parallel to the incident rays, but with a phase difference of π . They will thus cause a reduction of the intensity of the incident beam, which does not occur when the crystal is not in a reflecting position. There will, of course, be multiple reflections, some of which will be in phase with the incident beam, but the total effect is a reduction of intensity. Although within a very narrow angular range there is total reflection, the integrated intensity of the reflected beam is weakened compared with the reflection from a mosaic crystal. This is called primary extinction. This simple picture is reasonably adequate for the so-called Bragg case; but when both incident and reflected beams emerge on the same side of the crystal (the so-called Laue case) or when the crystal is completely bathed in the primary beam, the situation is more complicated.

Primary extinction occurs only in regions of a crystal which are perfect enough for exact phase relationships to apply. If the various parts are slightly out of register the phase differences are no longer exact, and amplitudes cannot be algebraically added or subtracted.

5.4.1. Distinction between Perfect and Ideally Imperfect Crystals

To decide whether the mosaic blocks in a crystal are small enough for a crystal to be considered ideally imperfect it is necessary to consider the amplitude of

the radiation reflected by a single plane of atoms. If q is this amplitude, the condition that primary extinction should be absent is that the number of planes m in a mosaic block should be such that mq is much less than unity. For example, for the 200 reflection from rock salt $q = 2.02 \times 10^{-4}$; hence m should be less than 500, corresponding to a thickness of 1400 Å. For the 400 reflection $q = 6.15 \times 10^{-5}$ and m should be less than 1600, corresponding to a thickness of 4600 Å.

5.4.2. Primary Extinction

It can be seen from the previous section that the size of crystals necessary for primary extinction to be negligible is smaller than is usually attainable, even in a fine powder. Because of the strength of the reflections it gives, rock salt is not typical, but even for more general crystals it is difficult to produce a specimen fine enough for primary extinction to be absent.

When the condition that mq should be much less than unity does not obtain, the quantity Q in equations 5.5 (1)–(11) must be replaced by a quantity such as Q' , where (Darwin [45])

$$\frac{Q'}{Q} = \frac{\tanh mq}{mq} \dots (1)$$

Values of $(\tanh mq)/mq$ are given in Table 5.4.2.

TABLE 5.4.2

Primary Extinction Correction Factor

mq	0.2	0.4	0.6	0.8	1.0
$(\tanh mq)/mq$..	0.971	0.949	0.896	0.832	0.761
mq	1.5	2.0	3.0	4.0	5.0
$(\tanh mq)/mq$..	0.604	0.482	0.332	0.250	0.200

Primary extinction can affect intensities from both single crystals and powders.

5.4.3. Secondary Extinction

Secondary extinction can occur together with primary extinction, but is different in nature. The mosaic blocks of a crystal may be small enough for the effects of primary extinction to be negligible, but the upper blocks in a crystal, by reflecting the radiation, may shield the lower ones, which will not therefore give their full contribution (W. H. Bragg [40]).

The effect can be allowed for by adding to the ordinary absorption coefficient μ a quantity gQ , where g is constant for a given crystal (Darwin [45]), but may vary considerably from specimen to specimen. No satisfactory way of determining g is known, although it may be derived from the experimental results if the structure is known.

It is sometimes possible to estimate the true structure factor by using a series of successively thinner or smaller crystals (Bragg, James and Bosanquet [41], Cochran [43]) and the mosaicity may sometimes be increased and extinction reduced by a thermal shock in liquid air or nitrogen. Methods have been suggested for estimating the perfection of a crystal (Ramaseshan and Ramachandran [46]) and of eliminating primary and secondary extinction simultaneously, by the use of polarized X-rays (Chandrasekhar [42]).

5.5. Summary of Formulae for Integrated Intensities

(a) Crystal Element

$$\rho = Q\delta V = \frac{N^2 e^4 \lambda^3 \delta V}{2m^2 c^4} \frac{1 + \cos^2 2\theta}{\sin 2\theta} |F|^2 \quad \dots (1)$$

(b) Crystal Face

1. Symmetrical Reflection

$$\rho' = \frac{Q}{2\mu} = \frac{N^2 e^4 \lambda^3}{4\mu m^2 c^4} \frac{1 + \cos^2 2\theta}{\sin 2\theta} |F|^2 \quad \dots (2)$$

2. Asymmetrical Reflection, when the reflecting planes are inclined at angle ϕ to the crystal face, and the face normal is in the plane of the incident and reflected beams.

Case (i) Angle of incidence $(\theta + \phi)$ and angle of emergence $(\theta - \phi)$

$$\rho' = \frac{Q}{2\mu} (1 - \cot \theta \tan \phi) \quad \dots (3)$$

Case (ii) Angle of incidence $(\theta - \phi)$ and angle of emergence $(\theta + \phi)$

$$\rho' = \frac{Q}{2\mu} (1 + \cot \theta \tan \phi) \quad \dots (4)$$

(c) Crystal Section of Thickness t

Reflecting planes perpendicular to surface:

$$\rho' = Qt \sec \theta \exp(-\mu t \sec \theta) = \frac{N^2 e^4 \lambda^3 t}{4m^2 c^4} \frac{1 + \cos^2 2\theta}{\sin \theta \cos^2 \theta} \exp(-\mu t \sec \theta) |F|^2 \quad \dots (5)$$

(d) Powder Halo: no absorption correction included

$$\frac{P}{I_0} = \frac{Qp''V \cos \theta}{2} = \frac{N^2 e^4 \lambda^3 V}{8m^2 c^4} \frac{1 + \cos^2 2\theta}{\sin \theta} p'' |F|^2 \quad \dots (6)$$

where P is the diffracted power.

(e) Debye-Scherrer Lines on Cylindrical Film: no absorption correction included

$$\frac{P_l}{I_0} = \frac{Qp''lV}{8\pi r \sin \theta} = \frac{N^2 e^4 \lambda^3 lV}{32\pi m^2 c^4 r} \frac{1 + \cos^2 2\theta}{\sin^2 \theta \cos \theta} p'' |F|^2 \quad \dots (7)$$

where l is the length of line measured and r is the radius of the camera. P_l is the power reflected into length l .

(f) Reflection from a Thick Block of Powdered Crystal of negligible transmission

$$\frac{P_l}{I_0} = \frac{Qp''l}{16\pi \mu r \sin \theta} = \frac{N^2 e^4 \lambda^3 l}{64\pi m^2 c^4 \mu r} \frac{1 + \cos^2 2\theta}{\sin^2 \theta \cos \theta} p'' |F|^2 \quad \dots (8)$$

(g) Transmission through Block of Powdered Crystal of Thickness t

$$\begin{aligned} \frac{P}{I_0} &= \frac{Qp''lt}{4\pi r \sin 2\theta} \frac{\delta'}{\delta} \\ &= \frac{N^2 e^4 \lambda^3}{8\pi m^2 c^4} \frac{lt\delta'}{\delta} \frac{1 + \cos^2 2\theta}{\sin 2\theta} p'' |F|^2 \quad \dots (9) \end{aligned}$$

where δ' , δ are the densities of the block of powder and of the crystal in bulk respectively.

(h) Rotation Photograph of Small Crystal, Volume V

1. Beam normal to axis, where ϕ is the angle between the axis of rotation and the reflecting plane,

$$\begin{aligned} \rho &= \frac{QVp'}{2\pi(\cos^2 \phi - \sin^2 \theta)^{\frac{1}{2}}} \\ &= \frac{N^2 e^4 \lambda^3 V}{4\pi m^2 c^4} \frac{1 + \cos^2 2\theta}{\sin 2\theta} \frac{1}{(\cos^2 \phi - \sin^2 \theta)^{\frac{1}{2}}} p' |F|^2 \quad \dots (10) \end{aligned}$$

2. Equi-inclination Weissenberg photograph:

$$\rho = \frac{QV}{2\pi \xi \cos \theta} = \frac{N^2 e^4 \lambda^3 V}{4\pi m^2 c^4} \frac{1 + \cos^2 2\theta}{\xi \cos \theta} |F|^2 \quad \dots (11)$$

Absorption is neglected in both (g) and (h).

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Section 6

FOURIER SYNTHESIS AND
STRUCTURE FACTORS

D. W. J. CRUICKSHANK

	PAGE
6.1. FORMULAE FOR THREE-DIMENSIONAL ELECTRON DENSITY AND PATTERSON FUNCTIONS (in collaboration with G. S. Parry)	318
6.2. FORMULAE FOR FOURIER SERIES, SECTIONS, LINES, PROJECTIONS AND DERIVATIVES .. (in collaboration with G. S. Parry)	319
6.3. FOURIER TRANSFORMS	322
6.4. REFINEMENT OF STRUCTURE PARAMETERS	326
6.5. THE PRACTICAL EVALUATION OF FOURIER SERIES AND STRUCTURE FACTORS (in collaboration with G. A. Jeffrey and P. J. Wheatley)	333

6.1. Formulae for Three-dimensional Electron Density and Patterson Functions

6.1.1. Electron Density

The Fourier series for the periodic variation of the electron density in a perfect infinite crystal is

$$\rho(XYZ) = \frac{1}{V_c} \sum_{h=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} F(hkl) \exp\{-2\pi i(hX + kY + lZ)\} \quad \dots (1)$$

where

$$F(hkl) = V_c \int_0^1 \int_0^1 \int_0^1 \rho(xyz) \exp\{2\pi i(hx + ky + lz)\} dx dy dz \quad \dots (2)$$

V_c is the volume of the unit cell, and (XYZ) and (xyz) are dimensionless fractional co-ordinates. If the unit cell axes are measured in Å, V_c has the dimensions of Å³, $\rho(XYZ)$ of electrons/Å³, and $F(hkl)$ of electrons/unit cell.

Let $F(hkl) = A'(hkl) + iB'(hkl)$, where A' and B' are real, and $\alpha(hkl) = \tan^{-1}(B'/A')$. Then, since $\rho(XYZ)$ is real:

$$A'(hkl) = V_c \int_0^1 \int_0^1 \int_0^1 \rho(xyz) \cos\{2\pi(hx + ky + lz)\} dx dy dz \quad \dots (3)$$

$$B'(hkl) = V_c \int_0^1 \int_0^1 \int_0^1 \rho(xyz) \sin\{2\pi(hx + ky + lz)\} dx dy dz \quad \dots (4)$$

$$\text{and} \quad F(hkl) = |F(hkl)| \exp\{i\alpha(hkl)\} \quad \dots (5)$$

By (3) and (4):

$$\begin{aligned} F(\bar{h}\bar{k}\bar{l}) &= A'(hkl) - iB'(hkl) \\ &= |F(hkl)| \exp\{-i\alpha(hkl)\} \end{aligned} \quad \dots (6)$$

$$\text{so that} \quad \alpha(\bar{h}\bar{k}\bar{l}) = -\alpha(hkl) \quad \dots (7)$$

$$\text{Further} \quad |F(\bar{h}\bar{k}\bar{l})| = |F(hkl)| \quad \dots (8)$$

[This is a formal consequence of definition (2) and the reality of $\rho(XYZ)$. Friedel's law of the same form relates to the amplitudes of the scattered waves, and may be explained on the assumption that these amplitudes are proportional to the right-hand side of (2). See Volume III for effects of anomalous scattering.]

Using (5) and (6), (1) may be written:

$$\rho(XYZ) = \frac{1}{V_c} \sum_{h=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} |F(hkl)| \cos\{2\pi(hX + kY + lZ) - \alpha(hkl)\} \quad \dots (9)$$

or alternatively

$$\begin{aligned} \rho(XYZ) &= \frac{1}{V_c} \sum_{h=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} \{A'(hkl) \cos 2\pi(hX + kY + lZ) \\ &\quad + B'(hkl) \sin 2\pi(hX + kY + lZ)\} \end{aligned} \quad \dots (10a)$$

If the crystal has a centre of symmetry at the origin, so that $F(hkl) = A'(hkl)$, (9) and (10a) reduce to

$$\rho(XYZ) = \frac{1}{V_c} \sum_{h=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} F(hkl) \cos 2\pi(hX + kY + lZ) \quad \dots (10b)$$

If the electron density is treated as a superposition of atomic electron densities

$$F(hkl) = \sum_t f_t(hkl) \exp\{2\pi i(hx_t + ky_t + lz_t)\} \quad \dots (11)$$

where the summation is over all the atoms of a unit cell, with co-ordinates (x_t, y_t, z_t) , and

$$f_t(hkl) = V_c \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \rho_t(uvw) \exp\{2\pi i(hu + kv + lw)\} du dv dw \quad \dots (12)$$

is the scattering factor of atom t whose electron density is $\rho_t(uvw)$, (uvw) being co-ordinates referred to (x_t, y_t, z_t) as origin. If the atomic densities are centrosymmetrical with respect to their origins the f_t are real and

$$A'(hkl) = \sum_t f_t(hkl) \cos\{2\pi(hx_t + ky_t + lz_t)\} \quad \dots (13)$$

$$\text{and} \quad B'(hkl) = \sum_t f_t(hkl) \sin\{2\pi(hx_t + ky_t + lz_t)\} \quad \dots (14)$$

are also real. If also the atomic densities have at least the symmetry of the crystal class, and in particular if they are spherically symmetrical,

$$A'(hkl) = \sum_r f_r(hkl) A(hkl) \quad \dots (15)$$

$$B'(hkl) = \sum_r f_r(hkl) B(hkl) \quad \dots (16)$$

where the summation is over the crystallographically non-equivalent atoms in the unit cell and

$$A(hkl) = \sum_s \cos\{2\pi(hx_s + ky_s + lz_s)\} \quad \dots (17)$$

$$\text{and} \quad B(hkl) = \sum_s \sin\{2\pi(hx_s + ky_s + lz_s)\} \quad \dots (18)$$

where the summation is over the atoms in the unit cell related to r by symmetry. *Note that (15) and (16) are not in general valid for non-spherical atoms, as symmetry-related atoms may then have different f 's.*

Volume I, Section 4.7, gives particular forms assumed by $\rho(XYZ)$, $A(hkl)$, and $B(hkl)$ in each space group.

6.1.2. The Patterson Function

By the convolution theorem (Section 2.5.3.1 and Table 2.5.4D), the Fourier series

$$P(UVW) = \frac{1}{V_c} \sum_{h=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} |F(hkl)|^2 \cos 2\pi(hU + kV + lW) \quad \dots (1)$$

involving only the amplitudes and not the phases of the structure factors, represents the function

$$P(uvw) = V_c \int_0^1 \int_0^1 \int_0^1 \rho(xyz) \rho(x+u, y+v, z+w) dx dy dz \quad \dots (2)$$

This function, introduced by A. L. Patterson [21] [22], gives a vectorial pattern of the distances between the atoms in a unit cell. On the use of the Patterson function see, for example, H. Lipson and W. Cochran [19].

6.2. Formulae for Fourier Series, Sections, Lines, Projections and Derivatives

The formulae in this section relate as they stand to the electron density. To make them applicable to the Patterson function, $|F(hkl)|$ must be replaced by $|F(hkl)|^2$, and α set equal to 0. The formulae are appropriate to the space group $P1$. To obtain the formulae for other space groups, corresponding modifications must be made to the electron density expressions given in Volume I, Section 4.7, or to the Patterson function expressions given in Volume I, Section 4.8 (which also lists the Harker sections). The arrangement of the expressions for computation is discussed in Section 6.5 (p. 333).

6.2.1. Electron Density Sections

6.2.1.1. For a plane parallel to (001), intersecting [001] at $Z=z_1$:

$$\rho(XYz_1) = \frac{1}{V_c} \sum_{h=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} |F(hkl)| \cos \{2\pi(hX+kY+lz_1) - \alpha(hkl)\} \quad \dots(1)$$

Since only one value of Z occurs it is easiest to evaluate this by summing first with respect to l . Thus, as a simple example, if there is a centre of symmetry at the origin, the section at $Z=\frac{1}{2}$ is

$$\rho(XY\frac{1}{2}) = \frac{1}{V_c} \sum_{h=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} C(hk) \cos 2\pi(hX+kY)$$

where
$$C(hk) = \sum_{l=-\infty}^{\infty} (-1)^l F(hkl).$$

The Patterson function always has a centre of symmetry at the origin and the Harker sections are always at values of X , Y or Z which are multiples of $\frac{1}{6}$, $\frac{1}{4}$, $\frac{1}{3}$ or $\frac{1}{2}$, so that they may always be evaluated by expressions resembling that given for $\rho(XY\frac{1}{2})$.

6.2.1.2. For a plane parallel to $(h_1k_1l_1)$, whose equation is

$$h_1X+k_1Y+l_1Z=p_1 \quad \dots(2)$$

$$\rho(XY)_{\text{plane}} = \frac{1}{V_c} \sum_{h=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} |F(hkl)| \cos \left\{ 2\pi \left[\left(h - \frac{h_1l}{l_1} \right) X + \left(k - \frac{k_1l}{l_1} \right) Y + \frac{lp_1}{l_1} \right] - \alpha(hkl) \right\} \quad \dots(3)$$

It should be noted that the area of the repeat unit of this expression is the same as that of the repeat unit in the plane $(h_1k_1l_1)$. [(2) can be used to eliminate X , Y or Z from 6.1.1(9). It is usually most convenient to eliminate the variable with the smallest non-zero Miller index. The preceding equation is one of the three possible.]

6.2.2. Electron Density Lines

6.2.2.1. Along a line parallel to [001] intersecting (001) at x_1y_1 :

$$\rho(x_1y_1Z) = \frac{1}{V_c} \sum_{h=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} |F(hkl)| \cos \{2\pi(hx_1+ky_1+lZ) - \alpha(hkl)\} \quad \dots(1)$$

In evaluation it is convenient to sum first with respect to h and k .

6.2.2.2. For a line parallel to $[uvw]$ passing through the point $x_1y_1z_1$, whose equation is

$$\frac{X-x_1}{u} = \frac{Y-y_1}{v} = \frac{Z-z_1}{w}$$

$$\rho(Z)_{\text{line}} = \frac{1}{V_c} \sum_{h=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} |F(hkl)| \cos \left\{ 2\pi \left[hx_1+ky_1 - \frac{(hu+kv)}{w}z_1 + \frac{(hu+kv+lw)}{w}Z \right] - \alpha(hkl) \right\} \quad \dots(2)$$

The line density repeats only after traversing a distance equal to the repeat distance along $[uvw]$. (Any one of three pairs of variables XY , YZ , ZX may be eliminated from 6.1.1(9), leaving an equation in one variable only. The preceding equation is one of the three possible.)

6.2.3. Electron Density Projections

6.2.3.1. The contents of the whole unit cell may be projected parallel to [001] on to any plane not containing [001], giving a projected electron density:

$$\rho(XY) = \frac{V_c}{A} \int_0^1 \rho(XYZ) dZ$$

$$= \frac{1}{A} \sum_{h=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} |F(hk0)| \cos \{2\pi(hX+kY) - \alpha(hk0)\} \quad \dots(1)$$

where A is the area of the (001) face of the cell.

Projection on to the plane orthogonal to [001] is often preferred. For this, $A = V_c/c$, with axes $a' = a \sin \beta$, $b' = b \sin \alpha$. In either case, with the unit cell axes measured in Å, the dimensions of $\rho(XY)$ are electrons/Å² of the projection.

(1) is one of the three principal axis projections.

6.2.3.2. A projection parallel to $[uvw]$ may be used to give the projected electron density of a unit cell having $[uvw]$ as one axis. The $F(hkl)$ for such a projection belong to the zone $[uvw]$ and have indices satisfying

$$hu+kv+lw=0 \quad \dots(2)$$

Such projections are often conveniently evaluated with

respect to new axes, two of which are taken in the plane (*uvw*).

6.2.3.3. A bounded projection parallel, say, to [001] gives the projection of the contents of the cell between two values of *Z* on to any plane not containing [001]. Thus if the limits are $Z=z_1$ and $Z=z_2$, the bounded projection is

$$B_{z_1}^{z_2}(XY) = \frac{V_c}{A} \int_{z_1}^{z_2} \rho(XYZ) dZ \quad \dots (3)$$

where *A* is the area of the (001) face of the cell (reference [3]). Before integrating it is convenient to separate those terms in the electron density series with $l=0$, thus:

$$\begin{aligned} \rho(XYZ) = & \frac{1}{V_c} \sum_{h=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} |F(hk0)| \cos \{2\pi(hX+kY)-\alpha(hk0)\} \\ & + \frac{1}{V_c} \sum_{h=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} |F(hkl)| \cos \{2\pi(hX+kY+lZ)-\alpha(hkl)\} \end{aligned} \quad \dots (4)$$

On substituting (4) in (3) and integrating we get

$$\begin{aligned} B_{z_1}^{z_2}(XY) = & \frac{(z_2-z_1)}{A} \sum_{h=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} |F(hk0)| \cos \{2\pi(hX+kY)-\alpha(hk0)\} \\ & + \frac{1}{A} \sum_{h=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} \frac{1}{2\pi l} |F(hkl)| [\sin \{2\pi(hX+kY+lz_2)-\alpha(hkl)\} \\ & - \sin \{2\pi(hX+kY+lz_1)-\alpha(hkl)\}] \end{aligned} \quad \dots (5)$$

or

$$\begin{aligned} B_{z_1}^{z_2}(XY) = & \frac{(z_2-z_1)}{A} \sum_{h=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} |F(hk0)| \cos \{2\pi(hX+kY)-\alpha(hk0)\} \\ & + \frac{1}{A} \sum_{h=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} |F(hkl)| [C_l \sin \{2\pi(hX+kY)-\alpha(hkl)\} \\ & + S_l \cos \{2\pi(hX+kY)-\alpha(hkl)\}] \end{aligned} \quad \dots (6)$$

where

$$\left. \begin{aligned} C_l &= \frac{1}{2\pi l} (\cos 2\pi l z_2 - \cos 2\pi l z_1) \\ S_l &= \frac{1}{2\pi l} (\sin 2\pi l z_2 - \sin 2\pi l z_1) \end{aligned} \right\} \quad \dots (7)$$

The summation consists of two distinct parts, the first being similar to (1) (it is identical if $z_2-z_1=1$) while the second is little more elaborate than the trigonometric expansion of 6.1.1(9). The factors C_l and S_l are constant when l is constant, so that the first summations should be made with respect to l .

6.2.3.4. A number of parallel electron density sections may be projected on to a common plane. Let the planes be parallel to (001) and intersect [001] in z_1, z_2, \dots, z_n . Then the required density function is

$$\rho(XYZ_1) + \rho(XYZ_2) + \dots + \rho(XYZ_n) = \sum_{r=1}^n \rho(XYZ_r)$$

Substituting from 6.1.1(9):

$$\begin{aligned} \sum_{r=1}^n \rho(XYZ_r) = & \frac{1}{V_c} \sum_{h=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} |F(hkl)| [C_l \cos \{2\pi(hX+kY)-\alpha(hkl)\} \\ & - S_l \sin \{2\pi(hX+kY)-\alpha(hkl)\}] \end{aligned} \quad \dots (8)$$

where

$$\left. \begin{aligned} C_l &= \sum_{r=1}^n \cos 2\pi l z_r \\ S_l &= \sum_{r=1}^n \sin 2\pi l z_r \end{aligned} \right\} \quad \dots (9)$$

6.2.3.5. The contents of the unit cell may be projected in planes parallel to, say, (001) on to any line not parallel to (001), giving a projected electron density:

$$\begin{aligned} \rho(Z) &= \frac{V_c}{d} \int_0^1 \int_0^1 \rho(XYZ) dX dY \\ &= \frac{1}{d} \sum_{l=-\infty}^{\infty} |F(00l)| \cos \{2\pi l Z - \alpha(00l)\} \end{aligned} \quad \dots (10)$$

where d is the length of the unit cell in the projection. With d in Å, the dimensions of $\rho(Z)$ are electrons/Å.

6.2.4. Differential Syntheses

The preceding formulae are often used to find the positions of the maxima of the electron density by interpolation from density values computed at regular intervals. An alternative method [5] of finding the position of a maximum is to compute the first and second derivatives of the electron density at a point (xyz) assumed near the maximum. The small shifts ($\epsilon_x, \epsilon_y, \epsilon_z$) to give the maximum at $(x+\epsilon_x, y+\epsilon_y, z+\epsilon_z)$ are determined by the following equations:

$$\left. \begin{aligned} \frac{\partial^2 \rho}{\partial x^2} \epsilon_x + \frac{\partial^2 \rho}{\partial x \partial y} \epsilon_y + \frac{\partial^2 \rho}{\partial x \partial z} \epsilon_z &= -\frac{\partial \rho}{\partial x} \\ \frac{\partial^2 \rho}{\partial x \partial y} \epsilon_x + \frac{\partial^2 \rho}{\partial y^2} \epsilon_y + \frac{\partial^2 \rho}{\partial y \partial z} \epsilon_z &= -\frac{\partial \rho}{\partial y} \\ \frac{\partial^2 \rho}{\partial x \partial z} \epsilon_x + \frac{\partial^2 \rho}{\partial y \partial z} \epsilon_y + \frac{\partial^2 \rho}{\partial z^2} \epsilon_z &= -\frac{\partial \rho}{\partial z} \end{aligned} \right\} \quad \dots (1)$$

where for the space group $P1$

$$\begin{aligned} \rho(xyz) &= \frac{1}{V_c} \sum_{h=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} |F(hkl)| \cos \{2\pi(hx+ky+lz)-\alpha(hkl)\} \\ \frac{\partial \rho}{\partial x} &= -\frac{2\pi}{V_c} \sum_{h=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} h |F(hkl)| \sin \{2\pi(hx+ky+lz)-\alpha(hkl)\} \end{aligned} \quad \dots (2)$$

with similar expressions for $\partial\rho/\partial y$ and $\partial\rho/\partial z$; and

$$\frac{\partial^2\rho}{\partial x\partial y} = -\frac{4\pi^2}{V_c} \sum_{h=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} hk |F(hkl)| \cos \{2\pi(hx+ky+lz) - \alpha(hkl)\} \dots (3)$$

with similar expressions for $\partial^2\rho/\partial y\partial z$, $\partial^2\rho/\partial x\partial z$, $\partial^2\rho/\partial x^2$, $\partial^2\rho/\partial y^2$ and $\partial^2\rho/\partial z^2$.

For other space groups, simplified expressions may be obtained by differentiating the appropriate expressions for the electron density given in Volume I, Section 4.7.

It is often convenient to specify co-ordinates in Å (or other suitable units) instead of axial fractions, as the principal second derivatives then have a more direct physical significance, values for similar atoms being affected only by thermal vibrations and the number of terms in the summation. Let (xyz) specify the co-ordinates of (xyz) in Å, then (1), (2) and (3) become

$$\left. \begin{aligned} \frac{\partial^2\rho}{\partial x^2}\epsilon_x + \frac{\partial^2\rho}{\partial x\partial y}\epsilon_y + \frac{\partial^2\rho}{\partial x\partial z}\epsilon_z &= -\frac{\partial\rho}{\partial x} \\ \frac{\partial^2\rho}{\partial x\partial y}\epsilon_x + \frac{\partial^2\rho}{\partial y^2}\epsilon_y + \frac{\partial^2\rho}{\partial y\partial z}\epsilon_z &= -\frac{\partial\rho}{\partial y} \\ \frac{\partial^2\rho}{\partial x\partial z}\epsilon_x + \frac{\partial^2\rho}{\partial y\partial z}\epsilon_y + \frac{\partial^2\rho}{\partial z^2}\epsilon_z &= -\frac{\partial\rho}{\partial z} \end{aligned} \right\} \dots (4)$$

where ϵ_x , ϵ_y , ϵ_z are the shifts in Å and

$$\frac{\partial\rho}{\partial x} = \frac{1}{a} \frac{\partial\rho}{\partial x'}, \text{ and } \frac{\partial^2\rho}{\partial x\partial y} = \frac{1}{ab} \frac{\partial^2\rho}{\partial x'\partial y'}, \text{ etc. } \dots (5)$$

If the electron density peak is spherically symmetrical, the following relations hold among the second derivatives at the peak in a triclinic cell:

$$\left. \begin{aligned} \frac{\partial^2\rho}{\partial x^2} = \frac{\partial^2\rho}{\partial y^2} = \frac{\partial^2\rho}{\partial z^2} = \frac{\partial^2\rho}{\partial r^2} \text{ (say)} \\ \frac{\partial^2\rho}{\partial x\partial y} = \frac{\partial^2\rho}{\partial r^2} \cos \gamma, \frac{\partial^2\rho}{\partial y\partial z} = \frac{\partial^2\rho}{\partial r^2} \cos \alpha, \frac{\partial^2\rho}{\partial x\partial z} = \frac{\partial^2\rho}{\partial r^2} \cos \beta \end{aligned} \right\} \dots (6)$$

where r is any radius of the spherical peak, and α , β and γ are the interaxial angles. Thus, if the peak is assumed spherical, one non-zero second derivative gives the values of all the others and (4) simplifies to

$$\left. \begin{aligned} \epsilon_x + \epsilon_y \cos \gamma + \epsilon_z \cos \beta &= -\frac{\partial\rho}{\partial x} / \frac{\partial^2\rho}{\partial r^2} \\ \epsilon_x \cos \gamma + \epsilon_y + \epsilon_z \cos \alpha &= -\frac{\partial\rho}{\partial y} / \frac{\partial^2\rho}{\partial r^2} \\ \epsilon_x \cos \beta + \epsilon_y \cos \alpha + \epsilon_z &= -\frac{\partial\rho}{\partial z} / \frac{\partial^2\rho}{\partial r^2} \end{aligned} \right\} \dots (7)$$

The solutions of (7) are, with

$$\left. \begin{aligned} \phi &= \left(\frac{\partial^2\rho}{\partial r^2} \right) (1 + 2\cos\alpha\cos\beta\cos\gamma - \cos^2\alpha - \cos^2\beta - \cos^2\gamma), \\ -\phi\epsilon_x &= (1 - \cos^2\alpha) \frac{\partial\rho}{\partial x} + (\cos\alpha\cos\beta - \cos\gamma) \frac{\partial\rho}{\partial y} \\ &\quad + (\cos\alpha\cos\gamma - \cos\beta) \frac{\partial\rho}{\partial z} \\ -\phi\epsilon_y &= (\cos\alpha\cos\beta - \cos\gamma) \frac{\partial\rho}{\partial x} + (1 - \cos^2\beta) \frac{\partial\rho}{\partial y} \\ &\quad + (\cos\beta\cos\gamma - \cos\alpha) \frac{\partial\rho}{\partial z} \\ -\phi\epsilon_z &= (\cos\alpha\cos\gamma - \cos\beta) \frac{\partial\rho}{\partial x} + (\cos\beta\cos\gamma - \cos\alpha) \frac{\partial\rho}{\partial y} \\ &\quad + (1 - \cos^2\gamma) \frac{\partial\rho}{\partial z} \end{aligned} \right\} \dots (8)$$

For a monoclinic cell, with b as the unique axis, (7) becomes

$$\left. \begin{aligned} \epsilon_x + \epsilon_z \cos \beta &= -\frac{\partial\rho}{\partial x} / \frac{\partial^2\rho}{\partial r^2} \\ \epsilon_y &= -\frac{\partial\rho}{\partial y} / \frac{\partial^2\rho}{\partial r^2} \\ \epsilon_x \cos \beta + \epsilon_z &= -\frac{\partial\rho}{\partial z} / \frac{\partial^2\rho}{\partial r^2} \end{aligned} \right\} \dots (9)$$

with solutions

$$\left. \begin{aligned} \epsilon_x &= \left(-\frac{\partial\rho}{\partial x} + \frac{\partial\rho}{\partial z} \cos \beta \right) / \left(\frac{\partial^2\rho}{\partial r^2} \sin^2 \beta \right) \\ \epsilon_y &= -\frac{\partial\rho}{\partial y} / \frac{\partial^2\rho}{\partial r^2} \\ \epsilon_z &= \left(-\frac{\partial\rho}{\partial z} + \frac{\partial\rho}{\partial x} \cos \beta \right) / \left(\frac{\partial^2\rho}{\partial r^2} \sin^2 \beta \right) \end{aligned} \right\} \dots (10)$$

If all the axes are orthogonal, these reduce to

$$\left. \begin{aligned} \epsilon_x &= -\frac{\partial\rho}{\partial x} / \frac{\partial^2\rho}{\partial r^2} \\ \epsilon_y &= -\frac{\partial\rho}{\partial y} / \frac{\partial^2\rho}{\partial r^2} \\ \epsilon_z &= -\frac{\partial\rho}{\partial z} / \frac{\partial^2\rho}{\partial r^2} \end{aligned} \right\} \dots (11)$$

These simplified equations must be used with caution, as electron-density peaks are sometimes appreciably ellipsoidal: for accurate work (1) or (4) should be used.

The use of differential syntheses in refinement with allowance for finite series corrections and for phase angle refinement in non-centrosymmetric space groups is discussed further in Section 6.4.2.

6.3. Fourier Transforms (cf. Section 2.5.3)

Let (xyz) be the co-ordinates of a point in direct space defined by the vector

$$x\mathbf{a} + y\mathbf{b} + z\mathbf{c}$$

where \mathbf{a} , \mathbf{b} , \mathbf{c} are base vectors enclosing a volume V_c , and let $(\xi\eta\zeta)$ be the co-ordinates of a point in reciprocal space defined by the vector

$$\xi\mathbf{a}^* + \eta\mathbf{b}^* + \zeta\mathbf{c}^*$$

where \mathbf{a}^* , \mathbf{b}^* , \mathbf{c}^* are the reciprocal base vectors.

The Fourier transform of a density function $\rho(xyz)$ is the scattering function

$$f(\xi\eta\zeta) = V_c \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \rho(xyz) \exp\{2\pi i(\xi x + \eta y + \zeta z)\} dx dy dz \quad \dots (1)$$

The inverse Fourier transform is

$$\rho(xyz) = \frac{1}{V_c} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(\xi\eta\zeta) \exp\{-2\pi i(\xi x + \eta y + \zeta z)\} d\xi d\eta d\zeta \quad \dots (2)$$

If \mathbf{a} , \mathbf{b} , \mathbf{c} are orthogonal and of unit length, the co-ordinates are in length units and $V_c = 1$ disappears from the formulae.

This Section lists a number of useful Fourier transforms and transform techniques, the latter including treatments of diffraction effects (Section 6.3.2) and of the effects of crystal shape (Section 6.3.5). Reference should be made to Section 2.5.3 for the basic mathematics of Fourier transform theory.

6.3.1. Radial Electron Densities

In three dimensions, the electron density $\rho_3(r)$ for a distribution with spherical symmetry about the origin is related to the scattering factor $f(s)$ by

$$\rho_3(r) = \int_0^{\infty} 4\pi s^2 f(s) \frac{\sin 2\pi sr}{2\pi sr} ds \quad \dots (1)$$

where r is the radius in length units in direct space, and $s = 2 \sin \theta / \lambda$, the radius in reciprocal space.

If $U(r) = 4\pi r^2 \rho_3(r)$ is the radial electron density:

$$\frac{U(r)}{r} = \int_0^{\infty} 8\pi s f(s) \sin 2\pi sr ds \quad \dots (2)$$

This is sometimes used as a series in the form

$$\frac{U(r)}{r} = \frac{8\pi}{D^3} \sum_{n=1}^{\infty} n f(n) \sin \left(\frac{2\pi nr}{D} \right) \quad \dots (3)$$

where $f(n)$ is the scattering factor for the n th order spectrum from planes of spacing D .

The electron density in a two-dimensional projection is

$$\rho_2(r) = \int_0^{\infty} 2\pi s f(s) J_0(2\pi sr) ds \quad \dots (4)$$

where $J_0(2\pi sr)$ is the zero order Bessel function.

The electron density in a one-dimensional projection is

$$\rho_1(r) = \int_0^{\infty} 2f(s) \cos(2\pi sr) ds \quad \dots (5)$$

6.3.2. Diffraction Effects

When the upper limit of integration of 6.3.1(1), (4) and (5) is $s_0 = 2(\sin \theta_{\max})/\lambda$, point atoms with unit scattering factor, $f(s) = 1$, are represented by density functions as follows:

3 dimensions:

$$\tau_3(r) = \int_0^{s_0} 4\pi s^2 \frac{\sin 2\pi sr}{2\pi sr} ds = \frac{\sin 2\pi s_0 r}{2\pi^2 r^3} - \frac{s_0 \cos 2\pi s_0 r}{\pi r^2} = \frac{4\pi s_0^3}{3} \left(\frac{3(\sin m - m \cos m)}{m^3} \right) \quad \dots (1)$$

where $m = 2\pi s_0 r$.

2 dimensions:

$$\tau_2(r) = \int_0^{s_0} 2\pi s J_0(2\pi sr) ds = \frac{s_0 J_1(2\pi s_0 r)}{r} = \pi s_0^2 \left(\frac{2J_1(m)}{m} \right) \quad \dots (2)$$

1 dimension:

$$\tau_1(r) = \int_0^{s_0} 2 \cos(2\pi sr) ds = \frac{\sin 2\pi s_0 r}{\pi r} = 2s_0 \left(\frac{\sin m}{m} \right) \quad \dots (3)$$

Table 6.3.2 shows the values of $s_0 r$ for the first four zeros of $\tau_3(r)$, $\tau_2(r)$ and $\tau_1(r)$.

TABLE 6.3.2

		$\tau_3(r)$	$\tau_2(r)$	$\tau_1(r)$
First zero	.. $s_0 r =$	0.715	0.610	0.5
Second zero	..	1.230	1.116	1.0
Third zero	..	1.736	1.619	1.5
Fourth zero	..	2.238	2.120	2.0

Figure 6.3.2 (taken from R. W. James [14]), shows the functions

$$\frac{3(\sin m - m \cos m)}{m^3}, \quad \frac{2J_1(m)}{m} \quad \text{and} \quad \frac{\sin m}{m}$$

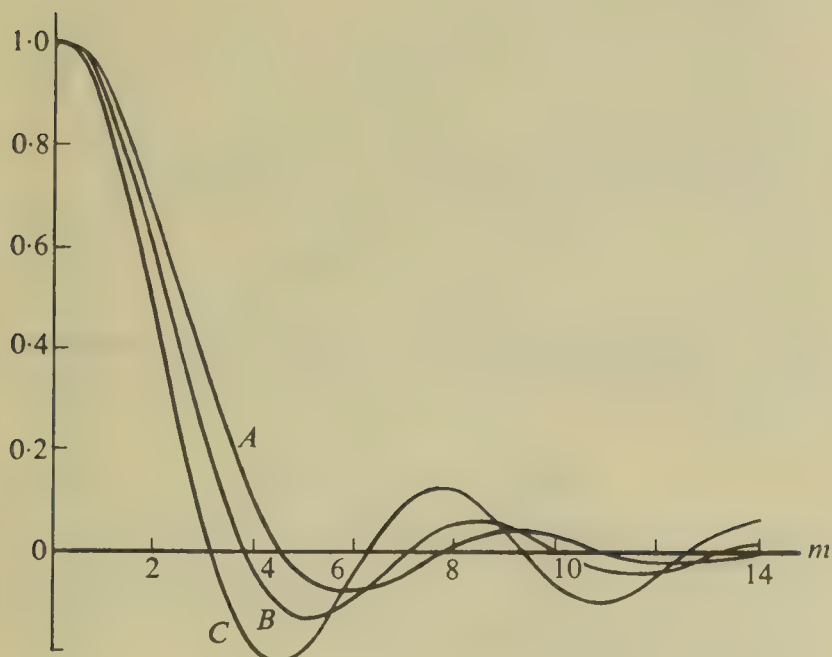


Fig. 6.3.2

Curves of (A), $3(\sin m - m \cos m)/m^3$; (B), $2J_1(m)/m$; (C), $(\sin m)/m$

The general effects of finite integration may be represented as follows. Suppose that the scattering function $f(\xi\eta\zeta)$ is observed only within a region S of reciprocal space. Then the density function $\rho(xyz)$ is replaced by

$$\psi(xyz) = \frac{1}{V_c} \int \int \int_S f(\xi\eta\zeta) \exp\{-2\pi i(\xi x + \eta y + \zeta z)\} d\xi d\eta d\zeta \quad \dots (4)$$

$$\text{Define } g(\xi\eta\zeta) = \begin{cases} 1 & \text{inside } S \\ 0 & \text{outside } S \end{cases}.$$

Then

$$\psi(xyz) = \frac{1}{V_c} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} f(\xi\eta\zeta) g(\xi\eta\zeta) \exp\{-2\pi i(\xi x + \eta y + \zeta z)\} d\xi d\eta d\zeta \quad \dots (5)$$

The inverse Fourier transform of $g(\xi\eta\zeta)$ is

$$G(xyz) = \frac{1}{V_c} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} g(\xi\eta\zeta) \exp\{-2\pi i(\xi x + \eta y + \zeta z)\} d\xi d\eta d\zeta \quad \dots (6)$$

Hence by the convolution theorem (Section 2.5.3.1, p. 66, and Table 2.5.4D, p. 82)

$$\psi(xyz) = V_c \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \rho(uvw) G^*(u-x, v-y, w-z) du dv dw \quad \dots (7)$$

Thus the finite integration density is obtained by multiplying the density at every point (uvw) by the function $V_c G^*(u-x, v-y, w-z)$ and integrating. When

S is a spherical region of reciprocal space, G^* is the function $\tau_3(r)$ of equation (1). Similarly, in two- and one-dimensional projections, G^* becomes $\tau_2(r)$ and $\tau_1(r)$.

Equation (7) also holds for the effect of finite summation on a periodic density function, if

$$g(\xi\eta\zeta) = \begin{cases} 1 & \text{for every observed lattice reflection } (hkl) \\ 0 & \text{for unobserved lattice reflections} \\ \text{arbitrary elsewhere} \end{cases}$$

This treatment of diffraction effects is the transform of the treatment of the effect of crystal shape given in Section 6.3.5.

6.3.3. Various Space Transforms

6.3.3.1. The scattering function $f(s)$ at reciprocal radius $s = 2 \sin \theta / \lambda$ of a distribution $\rho_3(r)$ with spherical symmetry about the origin is

$$f(s) = \int_0^{\infty} 4\pi r^2 \rho_3(r) \frac{\sin 2\pi sr}{2\pi sr} dr \quad \dots (1)$$

which is the inverse Fourier transform of 6.3.1(1).

6.3.3.2. For a plane distribution of circular symmetry of density $\rho_2(r)$ per unit area:

$$f(s) = \int_0^{\infty} 2\pi r \rho_2(r) J_0(2\pi tr) dr \quad \dots (2)$$

where t is the orthogonal projection of the reciprocal vector $s = (\xi\eta\zeta)$ on a reciprocal plane parallel to the distribution.

6.3.3.3. For a line distribution of density $\rho_1(r)$ per unit length:

$$f(s) = \int_{-\infty}^{\infty} \rho_1(r) \exp(2\pi itr) dr \quad \dots (3)$$

where t is the orthogonal projection of s on a line in reciprocal space parallel to the distribution.

6.3.3.4. Using (2) and (3), the scattering function for a distribution $\rho(R, z)$ of cylindrical symmetry, where z is the distance along the axis and R is the distance from the axis, is

$$f(t, \zeta) = \int_{-\infty}^{\infty} \left(\int_0^{\infty} 2\pi R \rho(R, z) J_0(2\pi tR) dR \right) \exp(2\pi i\zeta z) dz \quad \dots (4)$$

where ζ is the distance along the reciprocal axis parallel to z , and t is the distance from this axis.

6.3.3.5. Using (1), the scattering function for a spherically symmetric atom freely rotating spherically at radius r from a point (xyz) is

$$f(s) \exp\{2\pi i(\xi x + \eta y + \zeta z)\} \frac{\sin 2\pi sr}{2\pi sr} \quad \dots (5)$$

where s is the reciprocal radius of $(\xi\eta\zeta)$ and $f(s)$ is the scattering factor for the atom at rest.

6.3.3.6. Using (2), the scattering function for a spherically symmetric atom rotating about an axis at radius r from a centre (xyz) is

$$f(s)\exp\{2\pi i(\xi x + \eta y + \zeta z)\}J_0(2\pi tr) \quad \dots (6)$$

where t is the distance in reciprocal space from $(\xi\eta\zeta)$ to the axis through the origin parallel to the axis of rotation.

6.3.3.7. For the scattering from a hindered rotator, and for atoms uniformly distributed along a circular arc, see M. V. King and W. N. Lipscomb [16] and M. Atoji, T. Watanabé and W. N. Lipscomb [2].

6.3.3.8. For an exponentially decreasing density distribution

$$\rho_3(r) = \frac{N}{\pi} \left(\frac{p}{2}\right)^3 e^{-pr} \quad \dots (7)$$

the scattering function is

$$f(s) = \frac{N}{\{1 + (2\pi s/p)^2\}^2} \quad \dots (8)$$

where s is the reciprocal radius, p is an arbitrary parameter and N is the number of electrons in the distribution.

6.3.3.9. For a Gaussian density distribution

$$\rho_3(r) = N \left(\frac{p}{\pi}\right)^{\frac{3}{2}} e^{-pr^2} \quad \dots (9)$$

corresponding to

$$\rho_2(r) = N \left(\frac{p}{\pi}\right) e^{-pr^2} \quad \text{and} \quad \rho_1(r) = N \left(\frac{p}{\pi}\right)^{\frac{1}{2}} e^{-pr^2}$$

the scattering function is

$$f(s) = N e^{-\pi^2 s^2 / p} \quad \dots (10)$$

where s is the reciprocal radius, p is an arbitrary parameter and N is the number of electrons in the distribution.

6.3.3.10 The transform of an infinite helix of radius r and pitch P , defined with respect to rectangular axes by the equations

$$\left. \begin{aligned} x &= r \cos(2\pi z/P) \\ y &= r \sin(2\pi z/P) \\ z &= z \end{aligned} \right\} \quad \dots (11)$$

vanishes unless $\zeta = n/P$, where n is an integer and ζ is the distance along the reciprocal axis parallel to z . When $\zeta = n/P$ the transform is proportional to

$$f(t, \psi, n/P) = J_n(2\pi tr) \exp[i n(\psi + \pi/2)] \quad \dots (12)$$

where t is the distance from the ζ axis, ψ is the angle from the axis ξ (reciprocal to x) in the plane perpen-

dicular to the ζ axis, and $J_n(2\pi tr)$ is the Bessel function of order n .

If atoms of unit scattering factor are arranged on a helix with vertical spacing p between the atoms, the transform vanishes unless

$$\zeta = \frac{n}{P} + \frac{m}{p}$$

where m is an integer.

When P/p is a ratio of whole numbers and so

$$\zeta = \frac{n}{P} + \frac{m}{p} = \frac{l}{c} \quad (\text{say}) \quad \dots (13)$$

where l is an integer and c is the repeat distance along the z axis, the structure factor for the helical array of atoms is

$$F\left(t, \psi, \frac{l}{c}\right) = N \sum_n f\left(t, \psi, \frac{n}{P}\right) \quad \dots (14)$$

summed for all values of n solving (13), and $N = c/p$ is the number of atoms in the repeat distance and one atom is assumed to have $z = 0$.

Reference [8].

6.3.4. Molecular Transforms

The molecular transform $T(\xi\eta\zeta)$ of a molecule with atoms at (x_i, y_i, z_i) , having scattering factors f_i , is defined as

$$\begin{aligned} T(\xi\eta\zeta) &= \sum_i f_i \exp\{2\pi i(\xi x_i + \eta y_i + \zeta z_i)\} \\ &= \sum_i f_i \cos 2\pi(\xi x_i + \eta y_i + \zeta z_i) \\ &\quad + i \sum_i f_i \sin 2\pi(\xi x_i + \eta y_i + \zeta z_i) \\ &= A(\xi\eta\zeta) + iB(\xi\eta\zeta) \quad \dots (1) \end{aligned}$$

where $(\xi\eta\zeta)$ are the co-ordinates in the space reciprocal to (xyz) and the summation is over all atoms in the molecule.

As examples, the molecular transform of a plane hexagon ("benzene") consisting of six atoms, with unit scattering factors, lying in the xy plane with co-ordinates $\{\pm a, 0, 0\}$, $\{\pm a/2, \pm(\sqrt{3})a/2, 0\}$ is

$$T(\xi\eta\zeta) = 2 \cos 2\pi a\xi + 4 \cos \pi a\xi \cos \pi(\sqrt{3})a\eta \quad \dots (2)$$

and the transform of a tetrahedron with atoms at (a, a, a) , $(a, -a, -a)$, $(-a, a, -a)$, $(-a, -a, a)$ is

$$\begin{aligned} T(\xi\eta\zeta) &= 4 \cos 2\pi a\xi \cos 2\pi a\eta \cos 2\pi a\zeta \\ &\quad - 4i \sin 2\pi a\xi \sin 2\pi a\eta \sin 2\pi a\zeta \quad \dots (3) \end{aligned}$$

The molecular transform method can be helpful in solving crystal structures when the configurations of the constituent molecules may be assumed in advance. If there is only one independent molecule in the unit cell, the approximate crystal structure is solved by finding three co-ordinates of orientation (since the choice of origin is arbitrary). In principle this is done by rotating the molecular transform in the reciprocal

lattice until the moduli of the transform at the reciprocal lattice points agree with the structure factor amplitudes. Problems in systems of higher symmetry are attacked by combining the transforms of individual molecules.

The use of molecular transforms is simplified if the molecule is planar, as then the contours of the trigonometric part of the transform form cylinders, and the structure factors of any zone are obtained from sections through the cylinders. Their use is also simplified if some of the orientation co-ordinates are already known from other physical considerations.

The molecular transform method is useful in conjunction with the optical methods referred to in Section 6.5.4.

References: [17], [28], [6], [19].

6.3.5. Transforms of Crystal Shapes

The electron density of a finite perfect crystalline particle may be expressed as

$$\rho(xyz) = \rho_{\infty}(xyz)s(xyz) \quad \dots(1)$$

where $\rho_{\infty}(xyz)$ is the electron density of the infinite periodic crystal, represented by the Fourier series

$$\rho_{\infty}(xyz) = \frac{1}{V_c} \sum_{h=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} F(hkl) \exp\{-2\pi i(hx + ky + lz)\}$$

and $s(xyz) = \begin{cases} 1 & \text{inside the particle boundary} \\ 0 & \text{outside the particle boundary} \end{cases}$

is the shape function.

We define the shape transform of the crystalline particle as

$$\Psi(\xi\eta\zeta) = \frac{1}{V} S^*(\xi\eta\zeta) \quad \dots(2)$$

where V is the volume of the particle and $S^*(\xi\eta\zeta)$ is the inverse Fourier transform of $s(xyz)$. Hence

$$\Psi(\xi\eta\zeta) = \frac{V_c}{V} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} s(xyz) \exp\{-2\pi i(\xi x + \eta y + \zeta z)\} dx dy dz \quad \dots(3)$$

By the convolution theorem (Section 2.5.3.1, page 66, and Table 2.5.4D, page 82) the Fourier transform of the crystalline particle is

$$f(\xi\eta\zeta) = N \sum_{h=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} \sum_{l=-\infty}^{\infty} F(hkl) \Psi(h-\xi, k-\eta, l-\zeta) \quad \dots(4)$$

supposing that the particle has an integral number of unit cells

$$N = V/V_c \quad \dots(5)$$

Thus the Fourier transform of a crystalline particle is the shape transform repeated at each reciprocal lattice point (hkl) , multiplied by $NF(hkl)$.

Table 6.3.5 (adapted from Patterson [23]) shows the shape transforms for a number of types of particle in terms of variables

$$U_i = 2\pi M_i(h_i - \xi_i), \quad (i=1,2,3)$$

where $h_1=h$, $h_2=k$, $h_3=l$; $\xi_1=\xi$, $\xi_2=\eta$, $\xi_3=\zeta$, and where $M_1=x$, $M_2=y$, $M_3=z$ are the intercepts the particles make on the axes. The polyhedra are set with faces as shown. The axes for the ellipsoid coincide with the principal axes, and for the skew cylinder one axis coincides with the cylinder axis and the other two with the principal axes of the cross section.

References: [18], [23], [12], [28].

TABLE 6.3.5
Shape Transforms: $U_i = 2\pi M_i(h_i - \xi_i)$

Crystal Shape	Shape Transforms $\Psi(U_1 U_2 U_3)$	$N/(M_1 M_2 M_3)$
Parallelepiped {100}	$\prod_1^3 [\sin U_i / U_i]$	8
Octahedron {111}	$6 \sum_1^3 [U_i \sin U_i (U_k^2 - U_i^2)^{-1} (U_i^2 - U_j^2)^{-1}]$	4/3
Tetrahedron {111}	$3 \sum_1^3 \frac{U_i (i \cos U_i \sin U_j \sin U_k - \sin U_i \cos U_j \cos U_k)}{(U_k^2 - U_i^2)(U_i^2 - U_j^2)}$	8/3
Rhombic dodecahedron {110}	$\frac{16 \sum \{U_i \sin \frac{1}{2} U_i [\cos \frac{1}{2} U_i - \cos \frac{1}{2} U_j \cos \frac{1}{2} U_k]\}}{(U_1 + U_2 + U_3)(-U_1 + U_2 + U_3)(U_1 - U_2 + U_3)(U_1 + U_2 - U_3)}$	2
Ellipsoid	$3R^{-3}(\sin R - R \cos R); R^2 = U_1^2 + U_2^2 + U_3^2$	$4\pi/3$
Elliptic cylinder	$2(\rho U_3)^{-1} J_1(\rho) \sin U_3; \rho^2 = U_1^2 + U_2^2$	2π

6.4. Refinement of Structure Parameters

6.4.1. Application of the Method of Least Squares

6.4.1.1. NORMAL EQUATIONS

The method of least squares (Section 2.6.6.4) can be used in structure refinement (E. W. Hughes [13]) by minimizing some function of the observed and calculated intensities with respect to the structure parameters. The function most commonly used is

$$R_1 = \sum w(hkl) (|F_o(hkl)| - |F_c(hkl)|)^2 \quad \dots (1)$$

The function

$$R_2 = \sum w(hkl) (|F_o(hkl)|^2 - |F_c(hkl)|^2)^2 \quad \dots (2)$$

is also sometimes used. In (1) and (2) the summations are over the set of crystallographically independent observed planes, the w 's are the weights for each term, and F_o and F_c are the observed and calculated structure factors. To obtain the most accurate parameter values

$$w(hkl) = \frac{1}{\sigma^2(hkl)} \quad \dots (3)$$

where $\sigma^2(hkl)$ is the variance, or square of the standard deviation, of

$$(|F_o(hkl)| - |F_c(hkl)|) \quad \text{or} \quad (|F_o(hkl)|^2 - |F_c(hkl)|^2)$$

for R_1 or R_2 respectively.

To make the following description applicable either to R_1 or R_2 , we write

$$R = \sum w(hkl) \Delta^2(hkl) \quad \dots (4)$$

where $\Delta(hkl) = |F_o(hkl)| - |F_c(hkl)|$ for R_1

and $\Delta(hkl) = |F_o(hkl)|^2 - |F_c(hkl)|^2$ for R_2 .

Let u_1, u_2, \dots, u_n be the n parameters occurring in the $|F_c|$ whose values are to be determined. These parameters need not necessarily be atomic co-ordinates, but may include isotropic or anisotropic vibration parameters, site occupation factors, etc. If the value of any parameter, most commonly just a scale factor, needed to bring the $|F_o|$ to an absolute scale is unknown, it *must* be determined by introducing the appropriate inverse quantity as a parameter of the $|F_c|$. When the least-squares refinement has been completed the parameter is transferred back to the $|F_o|$.†

When R is a minimum,

$$\frac{\partial R}{\partial u_j} = 0, \quad (j=1, 2, \dots, n) \quad \dots (5)$$

$$\text{that is} \quad \sum w(hkl) \Delta(hkl) \frac{\partial \Delta(hkl)}{\partial u_j} = 0 \quad \dots (6)$$

The parameters must be chosen to satisfy these n conditions. For a trial set of values of the u_j close to the correct set, the normal equations for the corrections

ϵ_j to the parameters u_j , valid for small changes, are the n simultaneous linear equations

$$\sum_{i=1}^n \epsilon_i \left\{ \sum w(hkl) \frac{\partial \Delta(hkl)}{\partial u_j} \frac{\partial \Delta(hkl)}{\partial u_i} \right\} = - \sum w(hkl) \Delta(hkl) \frac{\partial \Delta(hkl)}{\partial u_j} \quad \dots (7)$$

($j=1, 2, \dots, n$)

where the $\partial \Delta(hkl)/\partial u_j$, etc., are evaluated for the trial parameter values. Note the minus sign on the right-hand side of (7).

$$\text{For } R_1: \quad \frac{\partial \Delta}{\partial u_j} = - \frac{\partial |F_c|}{\partial u_j}$$

$$\text{For } R_2: \quad \frac{\partial \Delta}{\partial u_j} = -2|F_c| \frac{\partial |F_c|}{\partial u_j}$$

Section 6.4.1.2 gives the values of $\partial |F_c|/\partial u_j$ for some common parameters. Note the minus sign in the relation between $\partial \Delta/\partial u_j$ and $\partial |F_c|/\partial u_j$.

The weights $w(hkl)$ are discussed in Section 6.4.1.3 and possible approximate forms of the equations in Section 6.4.1.4.

6.4.1.2. VALUES OF $\partial |F_c(hkl)|/\partial u_j$

(a) If u_j is a co-ordinate parameter of atom r , denoted by x_{ri} ($i=1,2,3$):

$$\frac{\partial |F_c(hkl)|}{\partial u_j} = \frac{\partial A_r(hkl)}{\partial x_{ri}} \cos \alpha + \frac{\partial B_r(hkl)}{\partial x_{ri}} \sin \alpha \quad \dots (8)$$

where A_r and B_r are the contributions of atom r and its symmetry equivalents to A' and B' ($F_c = A' + iB'$). For centrosymmetrical space groups $\sin \alpha = 0$, and

$$\frac{\partial |F_c(hkl)|}{\partial u_j} = \pm \frac{\partial A_r(hkl)}{\partial x_{ri}}$$

For spherically symmetrical atoms (or atoms having at least the symmetry of the crystal class)

$$A_r = f_r A \quad \text{and} \quad B_r = f_r B \quad \dots (9)$$

where A and B are given for the different space groups in Volume I, Section 4.7. Note that equations (9) are not in general valid for non-spherical atoms, as symmetry-related atoms may then have different f 's.

When the three co-ordinates of atom r are not independent, the differentiations $\partial A_r(hkl)/\partial x_{ri}$ and

† The reason for this is that if the $|F_o|$ are not fixed the criterion of minimum R is no longer appropriate. It is desirable instead to minimize some function of the proportionate discrepancies between the $|F_o|$ and the $|F_c|$: for instance, in place of R_1 the function

$$R_1 / \{ \sum w(hkl) |F_o(hkl)|^2 \}$$

The value of the scale factor, treated as a parameter of the $|F_o|$, obtained by minimizing this function is the same as that obtained from R_1 by the method indicated in the text.

$\partial B_r(hkl)/\partial x_{ri}$ must be made regarding x_{ri} as a parameter, and not simply as one of three unrelated co-ordinates (see Example 2).

EXAMPLES (for spherically symmetrical atoms)

1. $P2_1/c$. No. 14. Atom in general position.

$$k+l=2n \quad A=4 \cos 2\pi(hx+lz) \cos 2\pi ky; \quad B=0$$

$$k+l=2n+1 \quad A=-4 \sin 2\pi(hx+lz) \sin 2\pi ky; \quad B=0$$

$$A=B=0 \text{ if } h=l=0 \text{ or if } k=0$$

Hence

$$k+l=2n \quad \frac{\partial A_r}{\partial x} = -8\pi h f_r \sin 2\pi(hx+lz) \cos 2\pi ky$$

$$\frac{\partial A_r}{\partial y} = -8\pi k f_r \cos 2\pi(hx+lz) \sin 2\pi ky$$

$$\frac{\partial A_r}{\partial z} = -8\pi l f_r \sin 2\pi(hx+lz) \cos 2\pi ky$$

$$k+l=2n+1 \quad \frac{\partial A_r}{\partial x} = -8\pi h f_r \cos 2\pi(hx+lz) \sin 2\pi ky$$

$$\frac{\partial A_r}{\partial y} = -8\pi k f_r \sin 2\pi(hx+lz) \cos 2\pi ky$$

$$\frac{\partial A_r}{\partial z} = -8\pi l f_r \cos 2\pi(hx+lz) \sin 2\pi ky$$

2. $R\bar{3}m$. No. 166. Atom in special position (x, \bar{x}, z) . Hexagonal co-ordinates.

$$-h+k+l=3n \quad A=6\{\cos 2\pi[(h-k)x+lz] \\ + \cos 2\pi[(k-i)x+lz] \\ + \cos 2\pi[(i-h)x+lz]\}$$

$$-h+k+l=3n+1 \quad A=B=0$$

Hence

$$-h+k+l=3n$$

$$\frac{\partial A_r}{\partial x} = -12\pi f_r \{(h-k) \sin 2\pi[(h-k)x+lz] \\ + (k-i) \sin 2\pi[(k-i)x+lz] \\ + (i-h) \sin 2\pi[(i-h)x+lz]\}$$

$$\frac{\partial A_r}{\partial z} = -12\pi l f_r \{\sin 2\pi[(h-k)x+lz] \\ + \sin 2\pi[(k-i)x+lz] + \sin 2\pi[(i-h)x+lz]\}$$

(β) If u_j is the isotropic thermal parameter Q (usual notation B) common to all atoms, given by

$$F_c(hkl) = \exp\{-Q(\sin \theta/\lambda)^2\} F_c^0(hkl)$$

where $F_c^0(hkl)$ is the calculated structure factor without any temperature factor:

$$\frac{\partial |F_c(hkl)|}{\partial u_j} = -(\sin \theta/\lambda)^2 |F_c(hkl)| \quad \dots (10)$$

where $F_c(hkl)$ is the structure factor with the trial value of Q .

(γ) If u_j is the isotropic thermal parameter Q_r for atom r and its symmetry equivalents, given by

$$f_r = \exp\{-Q_r(\sin \theta/\lambda)^2\} f_r^0$$

where f_r^0 is the scattering factor for atom r at rest:

$$\frac{\partial |F_c(hkl)|}{\partial u_j} = \frac{\partial A_r(hkl)}{\partial Q_r} \cos \alpha + \frac{\partial B_r(hkl)}{\partial Q_r} \sin \alpha \\ = -(\sin \theta/\lambda)^2 \{A_r(hkl) \cos \alpha + B_r(hkl) \sin \alpha\} \quad \dots (11)$$

with A_r and B_r , defined by (9), calculated with the trial value of Q_r .

(δ) If u_j is one of the anisotropic thermal parameters for atom r , given by

$$f_r = \exp\{-(b_{11}h^2 + b_{12}hk + b_{13}hl + b_{22}k^2 + b_{23}kl + b_{33}l^2)\} f_r^0$$

where f_r^0 is the scattering factor for atom r at rest and if, for example, $u_j = b_{12}$:

$$\frac{\partial |F_c(hkl)|}{\partial b_{12}} = \frac{\partial A_r(hkl)}{\partial b_{12}} \cos \alpha + \frac{\partial B_r(hkl)}{\partial b_{12}} \sin \alpha \quad \dots (12)$$

where A_r and B_r are the contributions of atom r and its symmetry equivalents to A' and B' . In the space group $P1$:

$$A_r(hkl) = f_r \cos 2\pi(hx_r + ky_r + lz_r)$$

so that

$$\frac{\partial A_r(hkl)}{\partial b_{12}} = -hk f_r \cos 2\pi(hx_r + ky_r + lz_r) \quad \dots (13)$$

where f_r is calculated with the trial set of thermal parameters; similarly

$$\frac{\partial B_r(hkl)}{\partial b_{12}} = -hk f_r \sin 2\pi(hx_r + ky_r + lz_r) \quad \dots (14)$$

In other space groups

$$A_r(hkl) = \sum_s f_s \cos 2\pi(hx_s + ky_s + lz_s), \text{ etc.}$$

where the summation is over all atoms related to r by symmetry. Careful account must be taken of the differing dependencies of the symmetry-related atoms on the anisotropic parameters (see K. N. Trueblood [25]). Relations of the type (9) are not generally valid.

(ϵ) If u_j is the scale factor of $|F_o|$, given by

$$|F_o(hkl)| = a |F_o'(hkl)|$$

where $|F_o'|$ is the value of $|F_o|$ on an arbitrary scale, then as indicated in Section 6.4.1, a parameter $b=1/a$ must be introduced as a parameter of $|F_c|$, so that

$$|F_c(hkl)| = b |F_c'(hkl)|$$

where $|F_c'|$ is the value of $|F_c|$ when $b=1$. Consequently

$$\frac{\partial F_c(hkl)}{\partial b} = |F_c(hkl)| \quad \dots (15)$$

where $|F_c(hkl)|$ is the value of $|F_c|$ with the trial value of b .

When this scale factor b is required all the preceding derivatives (8), (10), (11), . . . , (14) must be multiplied by the trial value of b . To avoid the extra computation then involved the normal equations may alternatively be divided by b^2 for R_1 or b^4 for R_2 . This is equivalent to leaving the earlier derivatives unaltered, to taking an unscaled value of $|F_o(hkl)|$ on the right-hand side of (15) and in $\Delta(hkl)$, and to using

$$\Delta(hkl) = (1/b)|F_o(hkl)| - |F_c(hkl)|$$

for R_1 or to using

$$\Delta(hkl) = (1/b)^2 |F_o(hkl)|^2 - |F_c(hkl)|^2$$

for R_2 .

6.4.1.3. CHOICE OF WEIGHTS w

If $\sigma(|F_o| - |F_c|)$ is small in comparison with $|F_o|$,

$$\sigma^2(|F_o|^2 - |F_c|^2) = 4|F_o|^2 \sigma^2(|F_o| - |F_c|) \quad \dots (16)$$

so that the relation between the weights for R_1 and R_2 is

$$4|F_o(hkl)|^2 w_2(hkl) = w_1(hkl) \quad \dots (17)$$

With this relation and $\sigma(|F_o| - |F_c|)$ small, the parameters finally found by minimizing R_1 or R_2 differ only by amounts small compared with their standard deviations. It is thus only a matter of computational convenience as to whether R_1 or R_2 is minimized.

In practice absolute estimates of the weights are usually unknown in advance, and relative estimates must be made. In making these, account must be taken both of the accuracy of the $|F_o|$ and of the appropriateness of the calculated model on which the $|F_c|$ are based. The weights are often approximated by a simple function of $|F_o|$, since the absolute values of the uncertainties are frequently more strongly dependent on $|F_o|$ than on any other factor. The weights introduced by Hughes [13] are often used. These are

$$\left. \begin{aligned} w_1(hkl) &\propto \frac{1}{|F_o(hkl)|^2} \text{ for } |F_o| > 4|F_{\min}| \\ &\propto \frac{1}{16|F_{\min}|^2} \text{ for } |F_o| < 4|F_{\min}| \end{aligned} \right\} \quad \dots (18)$$

where $|F_{\min}|$ is the minimum observable $|F_o|$.

Care must be taken to see that a weighting scheme is appropriate. A good weighting scheme gives the least-squares method an advantage over the Fourier method in accuracy, but a bad one can give misleading conclusions.

6.4.1.4. APPROXIMATE EQUATIONS

The off-diagonal coefficients $\sum w \left(\frac{\partial \Delta}{\partial u_j} \right) \left(\frac{\partial \Delta}{\partial u_i} \right)$ of ϵ_i

in the normal equations (7) may often be neglected if

- (a) u_i is a co-ordinate parameter and u_j a scale or thermal parameter; accordingly the refinement of co-ordinates and scale parameters may be treated

independently, except that the thermal parameters of an atom with large vibrations may interact with the co-ordinates of its neighbours;

- (b) u_i and u_j are co-ordinate parameters of different atoms whose peaks do not overlap in the corresponding Fourier series, and if in a non-centrosymmetric space group the determination of the phases is not dominated by either of these atoms;
- (c) u_i and u_j are co-ordinate parameters in perpendicular directions of the same atom, whose Fourier series peak is spherical.

These approximations are most satisfactory when a large three-dimensional collection of data is used. Further details of the approximations possible for co-ordinate parameters will be found in D. W. J. Cruickshank [9].

The following interactions are always important and the corresponding off-diagonal coefficients should not be neglected:

- (a) The interaction between the scale parameter of $|F_o|$ and the overall thermal parameters of the structure;
- (b) The interactions between the anisotropic parameters b_{11} , b_{22} , and b_{33} of any atom; also the interactions involving b_{12} , b_{23} , and b_{13} when the corresponding axes are not nearly perpendicular;
- (c) The interaction between the co-ordinate parameters of any atom when the corresponding axes are not nearly perpendicular.

6.4.2. Refinement using Observed and Calculated Fourier Syntheses in Conjunction, or by Difference Syntheses

6.4.2.1. INTRODUCTION

Independently of the effects of experimental errors, the electron density given by a Fourier series of observed structure factors, $|F_o|$, differs from the true electron density because of the use of a finite series. Further, when the peaks overlap, the positions of the maxima of this finite series of observed electron density are not the required atomic positions. These difficulties may be largely overcome by using difference syntheses, having Fourier coefficients $(F_o - F_c)$, with terms present only where a corresponding F_o is present. Difference syntheses may be used to determine atomic co-ordinates, atomic scale and thermal parameters, to study the distribution of electrons in bonds or ionized atoms, and to locate light atoms. A difference synthesis is the difference of the finite series observed and calculated electron densities, and so these topics may alternatively be studied from separately computed observed and calculated syntheses used in conjunction. This section gives formulae for difference syntheses, and for the joint use of observed and calculated syntheses.

The usual criterion for determining atomic co-ordinates is that the slopes of the difference synthesis should be zero at the atomic positions, or equivalently that the slopes of the observed and calculated finite series electron densities should be equal.

The details of the refinement of scale and thermal parameters by difference syntheses will not be discussed (reference may be made to [7] and [10]), but possible criteria to be employed may be stated as follows. If the scattering factors for the atoms at rest are accurate, the six three-dimensional anisotropic thermal parameters of a given atom may be determined by the criteria that the six second derivatives of the difference synthesis should be zero at the atomic position. If the thermal motion is assumed isotropic, the single thermal parameter for an atom may be determined either from the criterion that the mean of the principal second derivatives of the difference synthesis should be zero or simply that the difference density itself should be zero at the atomic position. If there is in addition an uncertainty in the scale as well as in the thermal parameters, the criterion of zero difference density must be added to those of zero second derivatives. The refinement of co-ordinates by the equations discussed in the remainder of Section 6.4.2 is valid only if the scale and thermal parameters (which are needed for the $|F_c|$) are at least approximately correct.

When the refinement of a structure is incomplete, each kind of parameter error causes characteristic contour patterns in the difference synthesis. The interpretation of these contours is discussed in [19] and [15].

6.4.2.2. GENERAL CO-ORDINATE REFINEMENT EQUATIONS

$$\text{Let } \rho_o(xyz) = \frac{1}{V_c} \sum_h \sum_k \sum_l |F_o(hkl)| \cos \{2\pi(hx + ky + lz) - \alpha(hkl)\}$$

$$= \frac{1}{V} \sum \sum \sum |F_o| \cos(\theta - \alpha), \text{ say} \quad \dots (1)$$

$$\text{and } \rho_c(xyz) = \frac{1}{V} \sum \sum \sum |F_c| \cos(\theta - \alpha) \quad \dots (2)$$

The criterion determining the i th ($x_i = x, y, z$) co-ordinate of atom r is

$$\left(\frac{\partial(\rho_o - \rho_c)}{\partial x_i} \right)_r = 0, \text{ or } \left(\frac{\partial \rho_o}{\partial x_i} \right)_r = \left(\frac{\partial \rho_c}{\partial x_i} \right)_r \quad \dots (3)$$

the derivatives being evaluated at the position of atom r .

Equations for the simultaneous refinement of all co-ordinates may be derived from the first-order terms of the multivariate Taylor expansions in all parameters of each criterion (3). Let x_{ri} denote the i th co-ordinate

of atom r and ϵ_{ri} a small correction to it. The refinement equations are of the type

$$\sum_{s,j} \epsilon_{sj} \left\{ -\frac{2\pi}{V} \sum \sum \sum h_i \frac{\partial |F_c(hkl)|}{\partial x_{sj}} \sin(\theta - \alpha) \right\} = \left(\frac{\partial(\rho_o - \rho_c)}{\partial x_i} \right)_r \quad \dots (4)$$

$$\text{with } \frac{\partial |F_c(hkl)|}{\partial x_{sj}} = \frac{\partial A_s(hkl)}{\partial x_{sj}} \cos \alpha + \frac{\partial B_s(hkl)}{\partial x_{sj}} \sin \alpha \quad \dots (5)$$

where the summation $\sum_{s,j}$ is over the independent co-ordinate parameters x_{sj} , A_s and B_s are the contributions of atom s and its symmetry equivalents to A' and B' , and h_i is h, k or l as x_i is x, y or z . There is one equation of this type for each independent r, i . The equations are valid for small parameter changes.

For centrosymmetric space groups the equations reduce to

$$\sum_{s,j} \epsilon_{sj} \left\{ -\frac{2\pi}{V} \sum \sum \sum h_i \frac{\partial F_s}{\partial x_{sj}} \sin \theta_r \right\} = \left(\frac{\partial(\rho_o - \rho_c)}{\partial x_i} \right)_r \quad \dots (6)$$

$$\text{or } \sum_{s,j} \epsilon_{sj} \frac{\partial}{\partial x_{sj}} \left(\frac{\partial \rho_s}{\partial x_i} \right)_r = \left(\frac{\partial(\rho_o - \rho_c)}{\partial x_i} \right)_r \quad \dots (7)$$

where $F_s = A_s$, and $\rho_s(xyz)$ is the finite series calculated electron density of atom s and its symmetry equivalents.

The values of $\partial A_s(hkl)/\partial x_{sj}$ and $\partial B_s(hkl)/\partial x_{sj}$ are the same as those in Section 6.4.1.2(α). Only the right-hand sides of (4) and (6) are given by the difference synthesis. The coefficients on the left-hand side have to be computed separately.

The derivation of equations (4) and their close relation to the normal equations of least squares for the function R_1 are discussed in [9]. See also [7].

For examples of the non-approximate use of (4), see F. R. Ahmed and D. W. J. Cruickshank [1] for application to an unresolved projection, and M. R. Truter [26] for application in a non-centrosymmetric space group.

6.4.2.3. APPROXIMATE CO-ORDINATE REFINEMENT EQUATIONS, CENTROSYMMETRIC SPACE GROUPS

The coefficient of ϵ_{sj} in (7) is a function of ρ_s evaluated at the position of atom r . This coefficient may be neglected when the summation is such that the images of atom s and its equivalents do not appreciably overlap atom r . For $r \neq s$ this is usually the case in three-dimensional analyses, but the coefficient must not be neglected for unresolved peaks in projections. When none of the other atoms s appreciably overlap atom r , (7) becomes approximately

$$\sum_j \epsilon_{rj} \frac{\partial}{\partial x_{rj}} \left(\frac{\partial \rho_r}{\partial x_i} \right)_r = \left(\frac{\partial(\rho_o - \rho_c)}{\partial x_i} \right)_r \quad \dots (8)$$

where ρ_r is the finite series electron density due to atom r and its symmetry equivalents. The co-ordinates of

atom r are then determined by the three equations (8) with $x_i = x, y, z$.

If the image of atom r is not appreciably overlapped by any of its symmetry equivalents, (8) becomes

$$\sum_j \epsilon_{rj} \left(\frac{\partial^2 \rho_r}{\partial x_i \partial x_j} \right)_r = - \left(\frac{\partial(\rho_o - \rho_c)}{\partial x_i} \right)_r \quad \dots (9)$$

where ρ_r is now the finite series electron density due to atom r alone. As a series

$$\left(\frac{\partial^2 \rho_r}{\partial x_i \partial x_j} \right)_r = - \frac{4\pi^2}{V} \sum \sum \sum h_i h_j f_r \quad \dots (10)$$

where the summation is over all planes within the observed region of reciprocal space (and this includes planes which may have been systematically absent in the original space group).

As a further approximation the off-diagonal terms $(\partial^2 \rho_r / \partial x_i \partial x_j)_r$ with $i \neq j$ may be negligible when the (i, j) axes are perpendicular; each co-ordinate is then determined by a single equation.

6.4.2.4. BOOTH'S BACK-SHIFT METHOD FOR FINITE SERIES CORRECTION

In Booth's back-shift method [4] a synthesis is computed with coefficients F_c calculated for the co-ordinates of the maxima of the final observed synthesis, with terms present only where corresponding terms are present in the observed synthesis, and the finite series corrections are taken as the displacements to the maxima of the calculated synthesis with reversed signs. If differential syntheses are used these corrections are given by the equations (1) of Section 6.2.4 with the displacement signs reversed. In the present notation the shifts are given by

$$\sum_j \epsilon_{rj} \left(\frac{\partial^2 \rho_c}{\partial x_i \partial x_j} \right)_r = \left(\frac{\partial \rho_c}{\partial x_i} \right)_r \quad (x_i = x, y, z) \quad \dots (11)$$

At any stage of the refinement, the best co-ordinate shifts are the differences of the shifts of the observed and calculated syntheses. If the observed and calculated second derivatives are approximately equal, as they must be for Booth's method to be applicable, the shifts can be regarded as the solutions of the three equations,

$$\sum_j \epsilon_{rj} \left(\frac{\partial^2 \rho_c}{\partial x_i \partial x_j} \right)_r = - \left(\frac{\partial \rho_o}{\partial x_i} \right)_r + \left(\frac{\partial \rho_c}{\partial x_i} \right)_r = - \left(\frac{\partial(\rho_o - \rho_c)}{\partial x_i} \right)_r \quad (x_i = x, y, z) \quad \dots (12)$$

If the peak is spherical it may not be necessary to compute all six of the second derivatives on the left-hand side of the equations (12) (see Section 6.2.4).

The refinement equations (6) of the equal-slope criterion are more exact than (12), as they take full account of peak overlapping. The conditions of validity of Booth's method are those under which (6) may be reduced to (9), for then ρ_c will be nearly equal to ρ_r near the co-ordinate of atom r .

6.4.2.5. APPROXIMATE CO-ORDINATE EQUATIONS AND THE "n-SHIFT RULE," NON-CENTROSYMMETRIC SPACE GROUPS

The conditions under which the coefficient of ϵ_{sj} in 6.4.2(4), with $s \neq r$, may be neglected are the same as those for centrosymmetric space groups with the additional limitation that neither atom s nor atom r must dominate the determination of the phase angles α . If also the image of atom r is not appreciably overlapped by any of its symmetry equivalents, 6.4.2(4) reduces to

$$\sum_j \epsilon_{rj} \left\{ - \frac{4\pi^2}{V} \sum \sum \sum \frac{m}{2} h_i h_j f_r \right\} = - \left(\frac{\partial(\rho_o - \rho_c)}{\partial x_i} \right)_r \quad \dots (13)$$

where $m=1$ for the reflections with general α values, $m=2$ for the reflections with $\alpha=0$ or π , and the summation must include any planes systematically absent in the original space group within the reciprocal region of observation; such planes are given the same m values as those present in the same rows or zones. Comparison of (13) with (9) and (10) shows that shifts in the space group $P1$ are twice those of a centrosymmetric space group, and that for non-centrosymmetric space groups centred in some projections the shifts are between one and two times the centrosymmetric shifts, the exact multiple n depending on the space group. This is the "n-shift rule" introduced by D. P. Shoemaker, J. Donohue, V. Schomaker and R. B. Corey [24].

6.4.3. Standard Deviations of Structure Parameters

6.4.3.1. LEAST SQUARES

The normal equations 6.4.1(7) may be written

$$\sum_i \epsilon_i a_{ij} = b_j \quad \dots (1)$$

where

$$a_{ij} = \sum w \frac{\partial \Delta}{\partial u_i} \frac{\partial \Delta}{\partial u_j} \quad \dots (2)$$

and

$$b_j = - \sum w \Delta \frac{\partial \Delta}{\partial u_j} \quad \dots (3)$$

If $\sigma(u_j)$ is the standard deviation of u_j :

$$\sigma^2(u_j) = a^{jj} \quad \dots (4)$$

where a^{jj} is an element of the matrix (a^{ij}) inverse to (a_{ij}) . This result is applicable when the absolute weights are known.

If the weights are initially unknown, but their relative magnitudes can be assigned satisfactorily, the square of the standard deviation of an observation of unit weight may be estimated at the end of a refinement as

$$\Sigma w \Delta^2 / (m - n) \quad \dots (5)$$

where the w 's are the relative weights, the Δ 's have their final values and $(m - n)$ is the difference between the number of independent observations and the number of parameters determined. The estimated standard deviation $s(u_j)$ is then given by

$$s^2(u_j) = a^{jj} \left(\frac{\Sigma w \Delta^2}{m - n} \right) \quad \dots (6)$$

where a^{jj} is calculated from the matrix (a_{ij}) with the relative weights [cf. Section 2.6.6.4, (22a) and (23)].

Similarly the estimated covariance of u_i and u_j is

$$\text{cov}(u_i, u_j) = a^{ij} \left(\frac{\sum w \Delta^2}{m-n} \right) \dots (7)$$

6.4.3.2. FOURIER METHODS

The standard deviation of the density of a difference synthesis at a point (xyz) , assuming correct phase angles, is

$$\sigma\{\rho_o(xyz) - \rho_c(xyz)\} = \frac{1}{V} \left\{ \sum_{\text{independent}} \sigma^2\{F(hkl)\} \left[\sum_{\text{form}} \cos\{\theta - \alpha(hkl)\} \right]^2 \right\}^{\frac{1}{2}} \dots (8)$$

where $\sigma\{F(hkl)\}$ is the standard deviation of $F(hkl)$, the inner summation is over all planes of the same crystallographic form, the outer summation is over the independent F 's and $\theta = 2\pi(hx + ky + lz)$. At a general (xyz) position, if there are sufficient terms in the summation, this has the approximate value

$$\sigma(\rho_o - \rho_c) = \frac{1}{V} \left\{ \sum_{-h}^{+h} \sum_{-k}^{+k} \sum_{-l}^{+l} \sigma^2(F) \right\}^{\frac{1}{2}} \dots (9)$$

The standard deviation of the slope of a difference synthesis is usually required in electrons/Å⁴. The standard deviation of the x slope at a point (xyz) assuming correct phase angles is

$$\sigma\left(\frac{\partial(\rho_o - \rho_c)}{\partial x}\right) = \frac{1}{V} \frac{2\pi}{a} \left\{ \sum_{\text{independent}} \sigma^2\{F(hkl)\} \left[\sum_{\text{form}} h \sin(\theta - \alpha) \right]^2 \right\}^{\frac{1}{2}} \dots (10)$$

At a general (xyz) position this has the approximate value

$$\sigma\left(\frac{\partial(\rho_o - \rho_c)}{\partial x}\right) = \frac{1}{V} \frac{2\pi}{a} \left\{ \sum_{-h}^{+h} \sum_{-k}^{+k} \sum_{-l}^{+l} h^2 \sigma^2(F) \right\}^{\frac{1}{2}} \dots (11)$$

Similar expressions hold for the y and z slopes.

These expressions for the slope errors may be used in conjunction with the equations of Section 6.4.2 to determine the standard deviations of co-ordinates found from difference syntheses or from the joint use of observed and calculated syntheses.

For an atom with a well-resolved spherical peak in an orthorhombic cell of a centrosymmetric space group

$$\left. \begin{aligned} \sigma(x) &= \sigma\left(\frac{\partial D}{\partial x}\right) \left/ \left| \frac{\partial^2 \rho}{\partial x^2} \right| \right. \\ \sigma(y) &= \sigma\left(\frac{\partial D}{\partial y}\right) \left/ \left| \frac{\partial^2 \rho}{\partial y^2} \right| \right. \\ \sigma(z) &= \sigma\left(\frac{\partial D}{\partial z}\right) \left/ \left| \frac{\partial^2 \rho}{\partial z^2} \right| \right. \end{aligned} \right\} \dots (12)$$

where $\sigma(x)$, $\sigma(y)$, $\sigma(z)$ are the co-ordinate standard deviations in Å, $\sigma(\partial D/\partial x)$ etc., are the slope standard

deviations, $D = \rho_o - \rho_c$, and $\partial^2 \rho/\partial x^2$ is the second derivative of the peak in electrons/Å⁵. If the back shift method, equation 6.4.2(12), has been used

$$\frac{\partial^2 \rho}{\partial x^2} = \frac{\partial^2 \rho_c}{\partial x^2}, \text{ etc.}$$

If equation 6.4.2(9) has been used, $\partial^2 \rho/\partial x^2$ is 6.4.2(10) in electrons/Å⁵, thus:

$$\frac{\partial^2 \rho}{\partial x^2} = -\frac{1}{V} \frac{4\pi^2}{a^2} \sum \sum \sum h^2 f_r \dots (13)$$

Care must be taken to see that an approximately correct temperature factor is used for f_r . If $\sigma(\partial D/\partial x) = \sigma(\partial D/\partial y) = \sigma(\partial D/\partial z)$, (12) also holds for triclinic and monoclinic cells.

In non-centrosymmetric space groups with co-ordinates determined by the n -shift rule, the above expressions for co-ordinate standard deviations hold with $\partial^2 \rho/\partial x^2$ replaced by

$$-\frac{1}{V} \frac{4\pi^2}{a^2} \sum \sum \sum \frac{m}{2} h^2 f_r \dots (14)$$

which is the coefficient of ϵ_{rx} in 6.4.2(13) in length units.

To use the above expressions for standard deviations it is first necessary to estimate the $\sigma\{F(hkl)\}$. A simple way of estimating the combined effect of the experimental errors in the F_o 's and the imperfections of the model used for the F_c 's is to take $\Delta F = ||F_o(hkl)| - |F_c(hkl)||$ as an estimate of $\sigma\{F(hkl)\}$. Estimates of the effects of various kinds of experimental errors may be obtained by studies of the agreement between sets of independent observations of the same set of intensities, of equivalent reflections and on different crystals of the same substance. Further discussion of the estimation of $\sigma(F)$ and of the equations for co-ordinate standard deviations can be found in [11] and [19].

6.4.3.3. BOND LENGTH AND BOND ANGLE STANDARD DEVIATIONS

The standard deviation of a bond length between two atoms whose co-ordinate errors are uncorrelated is

$$\sigma(l) = \{\sigma^2(A) + \sigma^2(B)\}^{\frac{1}{2}} \dots (15)$$

where $\sigma(A)$ and $\sigma(B)$ are the standard deviations of the co-ordinates of the two atoms along the direction of the bond.

If the bond is across a centre of symmetry:

$$\sigma(l) = 2\sigma(A) \dots (16)$$

If β is the angle formed at B between the bonds AB and BC , the errors of the three atoms being uncorrelated:

$$\sigma^2(\beta) = \frac{\sigma^2(A)}{AB^2} + \sigma^2(B) \left(\frac{1}{AB^2} - \frac{2 \cos \beta}{AB \cdot BC} + \frac{1}{BC^2} \right) + \frac{\sigma^2(C)}{BC^2} \dots (17)$$

where $\sigma(A)$ and $\sigma(C)$ are the standard deviations of A and C in the directions at right angles to AB and BC respectively, and $\sigma(B)$ is the standard deviation of B in the direction of the centre of the circle passing through A , B and C . If A and B are related by a centre of symmetry, $\sigma^2(\beta)$ is given by replacing A by the centre of symmetry O , which has no error, and using the half-length OA in place of AB .

6.4.4. The Discrepancy Index (or Residual)

The quantity

$$R = \frac{\sum ||F_o(hkl)| - |F_c(hkl)||}{\sum |F_o(hkl)|}$$

is often used to follow the refinement of a structure as a rough and ready indication of the progress made. It is not directly related to the probable errors and in no way replaces methods such as those of Section 6.4.3 for estimating final parameter standard deviations; but it has the great merit of being computed quickly, and long use has endowed it with some qualitative significance.

Several slightly different definitions of R have been used, differing according to their treatment of reflections too weak for observation and their allowance for the multiplicity of the $|F|$'s. As R is not a fundamental quantity, there is usually little point in taking account of multiplicity. The omission of the $|F_c|$'s for unobserved $|F_o|$'s in the early stages of an analysis may, however, be misleading. In the final stages this is less important. Published values of R should be accompanied by a statement as to whether the unobserved planes were included or not. It is essential that the observed and calculated F 's are at least approximately on the same scale, so that $\sum |F_o(hkl)| \simeq \sum |F_c(hkl)|$.

A. J. C. Wilson [27] has shown that the value of R when the F_c 's are calculated for atoms in random position is 0.828 in centrosymmetric space groups and 0.586 in non-centrosymmetric space groups.

V. Luzzati [20] has discussed the variation of R , summed for groups of planes of approximately equal $\sin \theta/\lambda$, with the mean square co-ordinate error and with $\sin \theta/\lambda$, assuming no experimental errors in the $|F_o|$'s.

6.5. The Practical Evaluation of Fourier Series and Structure Factors†

With the extension of crystal structure analysis to many-parameter problems and the increasing use of quantitative measurement of X-ray intensities, the value of the Fourier synthesis was fully realized some fifteen years after the original suggestion by W. H. Bragg in 1915 [29]. The need for computational aids in the calculation of Fourier series and structure factors dates from about that time, for until practical methods for doing the extensive calculations had been evolved the subject could not proceed very far in certain directions.

Computational problems appear at two stages in a structure analysis: (1) in the solution of the phase problem and (2) in the refinement of the analysis so as to make the fullest use of the experimental data (Section 6.4). It would not be expected in general that a computational aid suitable for (1) would also be efficient for (2), where accuracy in dealing with a large quantity of data is a paramount requirement.

Crystallographic calculations can be done very rapidly and accurately on general-purpose electronic computing machines, but because of the need for specialized knowledge of programming and for the economical use of the limited number of machines available, some centralized planning of calculations may often be necessary. While centralized computing on general-purpose machines is likely to be employed increasingly for the calculations encountered in the final stages of refinement of analyses, there will probably always be a place for simpler aids to computation in the early stages of crystal analysis. For this reason, and because of their ready availability, a detailed account is given below of the Fourier strip methods, the Bragg-Lipson charts, and some optical methods.

6.5.1. The Fourier Strip Methods

Three methods of computing Fourier syntheses by means of strips which are commercially available or simple to construct are associated with the names Beevers-Lipson, Robertson, and Patterson-Tunell. They are commonly used only for one- and two-dimensional Fourier syntheses, as the calculations become very tedious for three-dimensional summations unless some specific sections and lines only are computed (Section 6.2) or a sampling method is used. However, as two-dimensional summations have already been described in some detail in Section 2.5.4 and as similar schemes are needed with punched-card or electronic computers, a three-dimensional example will be described now. The electron-density formulae must be rearranged for computation into a product form. If the space group Pm (Vol. I, page 377), with

b as unique axis, is taken as an example, the electron density formula becomes

$$\rho(XYZ) = \frac{4}{V_c} \left\{ \sum_{h=0}^{\infty} \sum_{k=0}^{\infty} \sum_{l=0}^{\infty} [\{A(hkl) + A(\bar{h}kl)\} \cos 2\pi hX \cos 2\pi kY \cos 2\pi lZ + \{-A(hkl) + A(\bar{h}kl)\} \sin 2\pi hX \cos 2\pi kY \sin 2\pi lZ + \{B(hkl) - B(\bar{h}kl)\} \sin 2\pi hX \cos 2\pi kY \cos 2\pi lZ + \{B(hkl) + B(\bar{h}kl)\} \cos 2\pi hX \cos 2\pi kY \sin 2\pi lZ] \right\}$$

where $A(hkl) = |F(hkl)| \cos \alpha(hkl)$

and $B(hkl) = |F(hkl)| \sin \alpha(hkl)$.

The summation may be carried out by an extension of the method already described for two-dimensional series in Section 2.5.4.7. Following the notation of that section we define

$$\begin{aligned} CCC(hkl) &= 4\{A(hkl) + A(\bar{h}kl)\} \\ SCS(hkl) &= 4\{-A(hkl) + A(\bar{h}kl)\} \\ SCC(hkl) &= 4\{B(hkl) - B(\bar{h}kl)\} \\ CCS(hkl) &= 4\{B(hkl) + B(\bar{h}kl)\} \end{aligned}$$

with appropriate care of the multiplicities when any index is 0 as described in Section 2.5.4.7, or in Vol. I, page 358. The calculation is carried out in three stages of one-dimensional Fourier summations.

If we define

$$f(XYZ) = V_c \rho(XYZ)$$

the electron density formula may be expressed as follows:

$$f(XYZ) = \sum_{k=0}^{\infty} C(XZ, k) \cos 2\pi kY \quad \dots (1)$$

$$\begin{aligned} \text{where } C(XZ, k) &= \sum_{l=0}^{\infty} CC(X, kl) \cos 2\pi lZ \\ &\quad + \sum_{l=1}^{\infty} CS(X, kl) \sin 2\pi lZ \quad \dots (2) \end{aligned}$$

$$\begin{aligned} \text{where } CC(X, kl) &= \sum_{h=0}^{\infty} CCC(hkl) \cos 2\pi hX \\ &\quad + \sum_{h=1}^{\infty} SCC(hkl) \sin 2\pi hX \quad \dots (3a) \end{aligned}$$

$$\begin{aligned} \text{and } CS(X, kl) &= \sum_{h=0}^{\infty} CCS(hkl) \cos 2\pi hX \\ &\quad + \sum_{h=1}^{\infty} SCS(hkl) \sin 2\pi hX \quad \dots (3b) \end{aligned}$$

The equations are evaluated in the reverse order: (3a) and (3b) first, then (2), and lastly (1); so that the summations over h are first and those over k are last.

† Most of the topics mentioned in this sub-section are discussed in detail and with examples in *The Determination of Crystal Structures*, by H. Lipson and W. Cochran [19].

As labour can be saved by using the symmetry properties (Section 2.5.4.5) of the one-dimensional cosine and sine series, it is wise to further subdivide the stages of the calculation. A calculation of the electron density for the complete asymmetric unit ($X=0 \rightarrow 1$, $Y=0 \rightarrow \frac{1}{2}$, $Z=0 \rightarrow 1$) might then be carried out in the following manner:

Stage 0. Combine the $A(hkl)$ and $A(\bar{h}kl)$, etc., to obtain the coefficients $CCC(hkl)$, etc., which appear on the r.h.s. of (3a) and (3b), making allowance for multiplicity where necessary. (If desired the factor 4 may be postponed until a later stage.)

Stage Ia. Divide the coefficients $CCC(hkl)$, etc., into groups with h even and h odd, and evaluate for $X=0 \rightarrow \frac{1}{4}$ (at intervals of, say, 1/60th) the eight summations

$$\sum_{(\text{even}) h=0}^{\infty} CCC(hkl) \cos 2\pi hX$$

$$\sum_{(\text{odd}) h=1}^{\infty} CCC(hkl) \cos 2\pi hX, \text{ etc.}$$

which appear on the r.h.s. of (3a) and (3b).

Stage Ib. Combine the results of the odd and even summations of Stage Ia and of the two summations on the r.h.s. of each of (3a) and (3b), in the manner of Section 2.5.4.7, to obtain the $CC(X,kl)$ and $CS(X,kl)$ for $X=0 \rightarrow 1$.

Stage IIa. Divide the $CC(X,kl)$ and $CS(X,kl)$ each into two groups with l even and l odd, and evaluate for $Z=0 \rightarrow \frac{1}{4}$ (and all X) the four summations

$$\sum_{(\text{even}) l=0}^{\infty} CC(X,kl) \cos 2\pi lZ, \text{ etc.}$$

which appear on the r.h.s. of (2).

Stage IIb. Combine the results of Stage IIa, in the manner of Section 2.5.4.7, to obtain the $C(XZ,k)$ for $Z=0 \rightarrow 1$ (and all X).

Stage IIIa. Divide the $C(XZ,k)$ into two groups with k even and k odd, and evaluate for $Y=0 \rightarrow \frac{1}{4}$ (and all X and Z) the summations

$$\sum_{(\text{even}) k=0}^{\infty} C(XZ,k) \cos 2\pi kY$$

and

$$\sum_{(\text{odd}) k=1}^{\infty} C(XZ,k) \cos 2\pi kY$$

which appear on the r.h.s. of (1).

Stage IIIb. Combine the results of Stage IIIa, in the manner of Section 2.5.4.7, to obtain $f(XYZ)$ for $Y=0 \rightarrow \frac{1}{2}$ (and all X and Z).

Comments

1. It is not necessary that the calculations in Stage I are completed for all values of X before Stages II and III are carried out. The above scheme is convenient with the strip methods, but for electronic computers of limited storage capacity there is no objection to

Stage I being carried out with a single value of X and the whole process repeated with the next value of X after obtaining the $f(X_1YZ)$.

2. Thought should always be given as to the best sequence of the summations in h , k and l . If the electron density is required throughout the asymmetric unit, the largest calculations usually arise in the Stage III summations, and consequently the last summation is ordinarily chosen to be for h , k or l according as to which of h_{\max} , k_{\max} or l_{\max} is least. However, in the above example, since no terms in $\sin 2\pi kY$ occur, the labour will probably be least if advantage of this is taken in Stage III (unless $k_{\max} > 2h_{\max}$ or $2l_{\max}$). If $h_{\max} > l_{\max}$ the summation in h should be in Stage I as shown.

6.5.1.1. THE BEEVERS-LIPSON STRIP METHOD

The values of the functions $C \cos 2\pi nhx$ and $C \sin 2\pi nhx$ are printed on two sets of strips (cosine and sine), each strip carrying the values of the function for a particular value of the amplitude C and order h , and all values of n . On the strips distributed prior to 1949, $2\pi x$ is 6° ($x=1/60$ th), n runs from 0 to 15, and the function is given to two figures. The numerical values of C run from 1 to 99, and of h from 0 to 20. The positive and negative values of a given amplitude are on front and back of the same strip (this is a convenient arrangement for making the sign changes at 15/60ths with cosines of odd order and sines of even order if it is desired to use the strips directly for values of x between 15/60ths and 30/60ths; all the strips are then read from right to left instead of left to right as ordinarily). The strips issued since 1949 have $x=1/120$ th and n from 0 to 30, with odd and even values of n on front and back of the same strip. C has values from ± 1 to ± 100 at intervals of 1 and thence to ± 900 in hundreds, with functions tabulated to the nearest whole number; h extends from 0 to 30.

For computation the appropriate strips for the value of C and h are selected from a box and the arguments are summed for each particular value of nx , usually with the aid of a desk adding machine.

These strips can also be used for calculating the geometric structure factors with co-ordinates defined to 6° or 3° intervals, and similarly for the calculation of Fourier transforms.

6.5.1.2. THE PATTERSON-TUNELL STRIP AND STENCIL METHOD

Values of $C \cos 2\pi nx$ are printed on cardboard strips with $2\pi nx$ extending from 0° to 90° in intervals of n with $x=1/60$ th or $1/48$ th. There is one strip for each integral value of C between ± 1 and ± 1000 , with the signs distinguished by white strips for positive values and coloured for negative. The arguments are accurate to whole numbers. The strips for each amplitude in the one-dimensional summation are arranged in order of their h values in a grooved rack. These

strips then form a table from which can be selected the values of $C \cos 2\pi hnx$ for each particular value of nx . This selection is done by means of a series of stencils which are placed over the strips in the racks and which permit only the appropriate figures to be seen through the holes. If a figure is seen through a hole which is ringed in colour, the sign of that figure must be reversed; thus, for example, a number on a coloured strip seen through a hole ringed in colour is positive.

Separate stencils are required for odd and even values of the order h and for each value of n from $nx=0$ to 0.250 , but opposite sides of the same stencil can be used for cosine and sine. For $x=6^\circ$, 32 stencils are required. Two stencils, one for odd h and one for even h , must be placed over the strips and the visible numbers summed to give $\sum_h C \cos 2\pi hnx$ for each value of nx .

6.5.1.3. ROBERTSON'S MODIFIED STRIP AND STENCIL METHOD

This is essentially the same as the Patterson-Tunell method, with the arguments on the strips in columns instead of rows. Each strip contains 31 numbers corresponding to $C \cos 2\pi nx$ for nx running from 0 to 0.250 with $x=1/120$ th. To avoid the dual signals for signs mentioned above, the sign of the amplitude is indicated by a small card which differentiates between positive and negative by the position of a red band. The appearance of this red band through additional holes in the stencils shows that the summation term is negative. Opposite sides of the same stencil can be used for the cosine and sine terms for the same values of nx .

A mechanical sorting device for use in conjunction with these strips has also been described.

See References [30]–[40].

6.5.2. The Bragg-Lipson Charts

In the early stages of a crystal analysis it is frequently useful to be able rapidly to obtain approximate values of principal zone structure factors. Bragg-Lipson charts enable the trigonometric components of the contributions of atoms to the structure factors to be derived graphically.

The charts are contour maps of the geometrical structure factors (Vol. I, p. 371). For considering only projection data, as is common practice, the seventeen plane groups can be covered by ten sets of maps. Each set will consist of a number of maps, one for each reflection in the particular zone under consideration. It is possible to make standard sets of these maps to cover all requirements, but it is more usual to select the sensitive "key" reflections in a particular zone and make the contour maps for those planes to scale for the particular unit cell dimensions. This procedure enables a model of the molecule to be placed on the

map and the contribution of each atom to the geometrical structure factor to be read off directly.

See Reference [41].

6.5.3. Mechanical and Electromechanical Methods

Many excellent computational aids have been invented which use a variety of principles and mechanical devices, and range from a simple slide-rule to complicated machines. Consultation of the original publication is necessary to construct these instruments and, in the case of the more complex machines, with the designer also. The bibliography is arranged so as to emphasize the principal objective of the method.

6.5.3.1. FOURIER SYNTHESIZERS

See References [42]–[49].

6.5.3.2. STRUCTURE FACTOR CALCULATORS

See References [50]–[60].

6.5.4. Optical Methods

There is a close analogy between X-ray diffraction and Fourier synthesis on the one hand and optical diffraction and image formation on the other. This similarity has been made the basis of a number of aids for structure analysis, but because of the difficulty of obtaining accuracy in these optical analogue methods they are chiefly directed towards the solution of the phase problem.

6.5.4.1. THE HUGGINS MASKS

A method originally suggested by W. L. Bragg has been systematized by Huggins [69], [70]. A cinematograph film of a set of masks with a density distribution given by $1 \pm \cos 2\pi(hX+kY)$ for different values of h and k is projected on to a sheet of photographic paper. Each mask is given an exposure proportional to $F(hk0)$. Providing that the total exposure is within the range of photographic proportionality, a Fourier synthesis is obtained on development of the photographic paper. The maximum and minimum density on the masks correspond to $\cos 2\pi(hX+kY)=+1$ and -1 respectively, and the positive and negative values of $F(hk0)$ are associated with the $1 - \cos 2\pi(hX+kY)$ and $1 + \cos 2\pi(hX+kY)$ masks respectively. The resultant Fourier pattern is consequently superimposed on a constant background of $\Sigma |F(hk0)|$.

6.5.4.2. THE "PHOTOSOMMATEUR" (G. v. Eller)

A versatile machine based on the same principle has been constructed by v. Eller [67]. A vertical slit source of light passing through a specially designed grating produces a sinusoidal distribution of intensity on a photographic plate mounted at the centre of a movable disc. The *intensity* depends on the exposure time, and the correct *orientation* of the Fourier terms relative to

each other is achieved by rotating the disc carrying the photographic plate. The *spacing* is altered by varying the distance between grating and source, the grating being geared to a cursor which permits the settings to be made directly from a drawing of the reciprocal lattice mounted on the rotating disc. The *phase* is introduced by an eccentric spindle which enables the grating which produces the vertical fringes to be translated horizontally by any amount up to one complete period 2π . It is thus just as easy to perform non-centrosymmetric summations as centrosymmetric ones.

Conversely, if a projection of the atoms in the unit cell is fixed to the machine in place of the reciprocal lattice, Fourier transforms can be prepared; and by inserting in the film holder a card punched with small holes at the positions of the reciprocal lattice points, spots whose blackening is proportional to $F(hk0)$ can be obtained. As with the Huggins masks, the density distribution recorded on the film is $1 + \cos 2\pi(hX + kY)$, so that the zero must be determined in order to decide whether $F(hk0)$ is positive or negative. This is done by sampling, side by side on the same film, the transforms prepared (a) for positive atoms and (b) for negative atoms.

6.5.4.3. THE X-RAY MICROSCOPE

If parallel monochromatic light is passed through a screen punched with holes to represent the magnitudes of the structure factors and their positions in the reciprocal lattice section, the image formed by focusing the emergent beam will be the Fourier synthesis of the diffraction pattern. This method can be used directly for the Patterson synthesis or for special cases of a Fourier synthesis when the phases are all the same. For general application to Fourier synthesis the phase differences must be introduced. This is done in the Buerger instrument by means of mica plates which are tilted to increase the optical path. In the Hanson and Lipson instrument the apertures in the screen represent only the reciprocal lattice positions, and the biaxial optical properties of mica are used to control both the amplitudes and the phases, which can only differ by integral multiples of π .

6.5.4.4. THE ANALOGUE DIFFRACTION SPECTROMETER

If the screen inserted in the beam of monochromatic light is punched with holes representing the position and X-ray scattering power of the atoms in a molecule, or projected view of a molecule, the image formed by focusing will be the Fourier transform of the molecule or projected molecule. This is the basis of an optical technique, due to Lipson and Taylor, for trial and error solution of the phase problem, and also for the study of the diffraction from imperfect structures.

If the screen transmits the light in a pattern corresponding to a large number of periodically repeated molecules, the Fourier transform is the diffraction

spectrum of the periodic structure. This forms the basis of the fly's-eye method, in which a suitable diffracting screen is made with a multiple-lens camera. The pattern produced by this screen is directly comparable with the experimental F^2 values for the appropriate zone of X-ray reflections.

Neither the Fourier-transform nor the fly's-eye method can indicate directly the phases of the diffracted pattern, but these can be determined in centrosymmetrical cases by observing the effect of introducing a heavy atom at the origin of the screen on the intensity of different parts of the transform or of the spectrum.

See References [61]–[77].

6.5.5. Large-scale Computing Equipment

Since the first edition of this Volume was published in 1959, the field of electronic computing as applied to crystallography has been growing so fast that it is useful only to give some of the main references.

6.5.5.1. COMPUTING METHODS

Reference [78] covers the proceedings of an International Summer School on Crystallographic Computing organised by the Commission on Crystallographic Computing of the International Union of Crystallography. Topics discussed include direct methods of phase determination, automatic interpretation of vector maps, utilisation of anomalous dispersion and isomorphous replacement, least-squares methods, analysis of atomic thermal vibration, absorption and extinction corrections, organisation of crystallographic computer systems, programs for computer-controlled diffractometers, and Fourier techniques. References [79] and [80] cover the proceedings of earlier meetings, many aspects of which remain relevant.

Attention is also drawn to Volume IV of these *International Tables*, in which some Sections are relevant to computing problems. The relevant Sections include those on angle settings for four-circle diffractometers, thermal motion analysis and direct methods.

6.5.5.2. LISTS OF PROGRAMS

Many programs are listed in the second edition of the *World List of Crystallographic Computer Programs* [81]. A third edition is in preparation by the Commission on Crystallographic Computing and is expected to be published in 1972–3.

6.5.5.3. TEST CALCULATIONS

It is not easy to ensure that complex computer programs are free from error. Accordingly the Commission on Crystallographic Computing have devised a series of calculations to check programs. These have been published in a report entitled "Standard Tests for Crystallographic Computer Programs, Part I.

Calculations used in Crystal Structure Analyses.” [82]. The test calculations include structure factors, interatomic distances and angles, Fourier syntheses and least-squares refinements.

Note: In Vol. IV (to be published in 1972) Sections 3, 4, 5, and 6 are computer-oriented mathematical sections, although they do not deal specifically with computing.

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Section 7

SPECIAL TOPICS

	PAGE
7.1. CLOSE PACKING (A. L. PATTERSON and J. S. KASPER)	342
7.2. THE USE OF STATISTICAL METHODS FOR THE DETECTION OF SYMMETRY ELEMENTS (V. LUZZATI)	355
7.3. INEQUALITY RELATIONS BETWEEN STRUCTURE FACTORS (J. BOUMAN)	358

7.1. Close Packing

By A. L. PATTERSON and J. S. KASPER

7.1.1. Introduction

The earliest known attempts to explain the regular external form of crystals made use of the notion of the close packing of spheres, and modern research has shown that such packing is of the greatest structural importance in many crystals. No attempt can be made in the space available to summarize the literature in a field of this importance. The tables of this section contain some of the available data on the close packing of circles in the plane and of spheres in space.

In the *close packing of circles in the plane* each circle has at least three contacts in the plane, and not all of these contacts fall in the same semicircle. In the *close packing of spheres in space* each sphere has at least four contacts to neighbouring spheres, and not all of these contacts fall in the same hemisphere. For a discussion of packing in space with less than four contacts reference is made to the literature (Heesch and Laves [4], Melmore [7]).

A *lattice packing* is one in which the packed objects are equivalent under the operations of a translation group. In *plane-group packing* and in *space-group packing* the packed objects are equivalent under the operations of a plane group and a space group respectively.

NOTE. In the following text it is assumed that the packed circles and spheres have *diameter unity*, and all dimensions must be interpreted accordingly.

7.1.2. Close Packing in the Plane

In the general lattice close packing in the plane, circles (diameter unity) occupy the special positions $0,0; \frac{1}{2}, \frac{1}{2}$ (Wyckoff notation $2(a)$; see Vol. I, p. 52, and Sections 4.2 and 4.3) of the plane group $c2mm$, with translations $a=2 \sin \gamma/2$ and $b=2 \cos \gamma/2$. Secondary contacts limit the parameter γ to the range defined by $-\frac{1}{2} < \cos \gamma < \frac{1}{2}$. The two special cases of lattice close packing of higher symmetry are listed in Table 7.1.2.

There are 33 plane-group packings (Niggli [11] [12], Haag [2] [3]) of circles in a plane. Two of these of high symmetry and of special interest are included in Table 7.1.2. There are at least 54 plane-group close-packed arrangements of ellipses in the plane (Nowacki [13]).

7.1.3. Close Packing in Space

In the general lattice close packing in space, spheres (diameter unity) occupy the special position $0,0,0$ (Wyckoff notation $1(a)$) of the space group $P\bar{1}$ with translations $a=b=c=1$ and angles α, β, γ which are arbitrary within ranges prescribed by secondary contacts (Minkowski, [9] [10]). There are fifteen lattice close packings of differing co-ordination number and symmetry which include ten of the Bravais lattices, excepting those of symmetry $P2/m, Pmmm, Fmmm$, and $P4/mmm$ (Patterson [14]). In Table 7.1.3 the five lattice close packings of spheres whose parameters are

TABLE 7.1.2
Some Close-packed Plane Arrangements of Circles

NOTATION							
Z=number of contacts per circle.							
S=cell area for circles of diameter unity.							
D=N/S=density in circles per unit area.							
C= $\pi D/4$ =fractional coverage of plane by circles.							
Z	Plane Group	Special Positions	a, b	S	D	C	Remarks
6	$p6m$	$1(a):0,0$	1	$\sqrt{3}/2$	$2/\sqrt{3}=1.1547$	0.9069	Closest plane packing†
4	$p4m$	$1(a):0,0$	1	1	1	0.7854	Square plane packing
3	$p6m$	$2(b):\frac{1}{3}, \frac{2}{3}; \frac{2}{3}, \frac{1}{3}$	$\sqrt{3}$	$3\sqrt{3}/2$	$4/3\sqrt{3}=0.7698$	0.6046	Triangular packing
3	$p6m$	$6(e)^\ddagger$	$2+\sqrt{3}$	$(12+7\sqrt{3})/2$	$4(7\sqrt{3}-12)=0.4974$	0.3906	Rarest close packing§

† This is the densest packing in the plane, and is unique.

‡ $x, \bar{x}; x, 2x; 2\bar{x}, \bar{x}; \bar{x}, x; \bar{x}, 2\bar{x}; 2x, x$; with $x=1-1/\sqrt{3}=0.4226$.

§ This is the rarest (least dense) possible plane-group packing and is probably the rarest close packing which will cover the plane.

7.1. CLOSE PACKING

TABLE 7.1.3

Some Close-packed Space Arrangements of Spheres

NOTATION

Z=number of contacts per sphere.

V=cell volume for spheres of diameter unity.

D=N/V=density in spheres per unit volume.

C=fractional coverage of space by spheres.

Z	Space Group	Special Positions (Wyckoff notation)	a, b, c	V	D	$C=\pi D/6$	Remarks
12	$Fm\bar{3}m$	4(a)	$\sqrt{2}$	$2\sqrt{2}$	$\sqrt{2}=1.4142$	0.7405	Cubic closest packing†
10	$I4/mmm$	2(a)	$\sqrt{(3/2)} (c=1)$	$3/2$	$4/3=1.3333$	0.6981	Body-centred tetragonal
8	$Im\bar{3}m$	2(a)	$2/\sqrt{3}$	$8/(3\sqrt{3})$	$(3\sqrt{3})/4=1.2990$	0.6801	Body-centred cubic
8	$P6/mmm$	1(a)	1	$\sqrt{3}/2$	$2/\sqrt{3}=1.1547$	0.6046	Simple hexagonal
6	$Pm\bar{3}m$	1(a)	1	1	1	0.5236	Simple cubic
4	$Fd\bar{3}m$	8(a)‡	$4/\sqrt{3}$	$64/(3\sqrt{3})$	$(3\sqrt{3})/8=0.6495$	0.3401	Diamond structure†
4	$Fd\bar{3}m$	32(e)‡§	$\frac{2}{3}[2\sqrt{3}+3\sqrt{2}]$	$\frac{16}{9}[22\sqrt{3}+27\sqrt{2}]$	$3[27\sqrt{2}-22\sqrt{3}]=0.2359$	0.1235	Rarest (?) packing†

† For generalizations of these packing types see 7.1.6.

‡ The origin is at the point of symmetry $\bar{4}3m$.

§ The value of the x parameter is $(3-\sqrt{6})/8=0.06881$.

completely determined by symmetry are presented. To these are added two space-group close packings of high symmetry and special interest. The number of space-group close packings of spheres is unknown (cf. Hilbert and Cohn-Vossen [5] [6] and Toth [16]).

7.1.4. Closest Packing of Spheres

The hexagonal packing of circles in the plane is clearly the closest possible planar packing, since each circle can have six neighbours in one and only one way, and this is also the largest possible number of nearest neighbours. A repetition of this arrangement covers the plane uniquely, so that the densest lattice close packing is also the closest packing for the plane.

It has been shown (Minkowski [9] [10]) that cubic closest packing is the densest lattice close packing of spheres, but so far it does not seem to have been proved that this is the closest possible packing of spheres which will fill space (cf. Toth [16]). The problem in space is complicated by the fact that there are infinitely many ways in which twelve spheres can be made to contact a single sphere. Among these there are two ways which when repeated in space lead to closest-packed planes of spheres. These two methods of arrangement of nearest neighbours lead to the

traditional closest-packing arrangements of spheres with a density of $\sqrt{2}$ spheres per unit of volume. In the sequel we shall use the term *closest packing of spheres* for the close-packed arrangements which contain closest-packed planes of spheres and possess the same density as the cubic-lattice closest packing of spheres (i.e. the face-centred cubic lattice). We recognize, however, that validity of the word “closest” in the heading and elsewhere in this sub-section is still in question. In particular, it has been shown that there are special arrangements of spheres (in a finite volume) with a density that exceeds that of the “closest-packed” arrangements (Boerdijk [1]). For example, a configuration of 33 spheres based on an icosahedral surrounding of a central sphere by its twelve neighbours has a smaller volume than that containing the same number of spheres in a “closest-packed” arrangement.

7.1.5. Symmetrical Closest-packed Stacking of Closest-packed Planes

The close-packed plane has sphere centres at one of the special points $1(a):0,0$; $1(b):\frac{1}{3},\frac{2}{3}$; or $1(c):\frac{2}{3},\frac{1}{3}$ of the plane group $p3m1$. In the following discussion a hexagonal cell of translation $a=1$ will be used for

spheres of diameter unity, while the c translation will be determined by the nature of the packing sequence.

A close-packed layer is said to be of type A when it has co-ordinates $0,0,z$. The next layer above it can be of type B with co-ordinates $\frac{2}{3},\frac{1}{3},z+c_0$ or of type C with co-ordinates $\frac{1}{3},\frac{2}{3},z+c_0$, where $c_0=\sqrt{\frac{2}{3}}=0.81650$ is the separation between two close-packed layers. Similarly, a B-layer may be followed by C or A, and a C-layer by A or B. A change from $A \rightarrow B \rightarrow C \rightarrow A$ for z increasing is called a positive change (+), while one from $A \rightarrow C \rightarrow B \rightarrow A$ is called negative (-). The translations corresponding to these changes and the locations and dimensions of the interlayer voids are given in Table 7.1.5A.

TABLE 7.1.5A

Interlayer Translations and Locations of Voids

Vectors give co-ordinates with respect to initial layer (A, B, or C) of layer above and of voids between the two layers ($c_0=\sqrt{\frac{2}{3}}=0.81650$).

Tetrahedral voids can contain a sphere of diameter $(\sqrt{\frac{3}{2}}-1)=0.2247$ which will be in contact with 4 spheres.

Octahedral voids can contain a sphere of diameter $(\sqrt{2}-1)=0.4142$ which will be in contact with 6 spheres.

Change	Translation	Tetrahedral Voids	Octahedral Void
+	$\frac{2}{3},\frac{1}{3},c_0$	$\frac{2}{3},\frac{1}{3},c_0/4$ $0,0,3c_0/4$	$\frac{1}{3},\frac{2}{3},c_0/2$
-	$\frac{1}{3},\frac{2}{3},c_0$	$\frac{1}{3},\frac{2}{3},c_0/4$ $0,0,3c_0/4$	$\frac{2}{3},\frac{1}{3},c_0/2$

It has been shown (Zhdanov [17]) that a given packing is characterized by a sequence of numbers each of which represents the number of repetitions or successions of a given sign for the change between layers, while the succeeding number then represents the number of successions of the opposite sign. Thus the symbol 2,2,12,6 would represent the successions 2 positive, 2 negative, 12 positive, 6 negative, this sequence then repeating indefinitely in a crystal packing. Clearly there must be an even number of numbers in such a symbol. If all such succession numbers are single digits the commas can be omitted: thus 2,2,4,4,6,2 would become 224462.

Let p be the number of positive signs and n be the number of negative signs in a given sequence. We then have

$$p+n=N \quad \dots(1)$$

where N is the number of layers in the period. Then if

$$p-n \equiv 0 \pmod{3} \quad \dots(2a)$$

the lattice will be hexagonal with $c=Nc_0$. If

$$p-n \equiv \pm 1 \pmod{3} \quad \dots(2b)$$

the lattice will be rhombohedral. For the two signs the three rhombohedral axes will have components in the hexagonal system as follows:

$$+ \text{ sign} \begin{pmatrix} \frac{2}{3},\frac{1}{3},Nc_0 \\ -\frac{1}{3},\frac{1}{3},Nc_0 \\ -\frac{1}{3},-\frac{2}{3},Nc_0 \end{pmatrix} \quad - \text{ sign} \begin{pmatrix} \frac{1}{3},\frac{2}{3},Nc_0 \\ -\frac{2}{3},-\frac{1}{3},Nc_0 \\ \frac{1}{3},-\frac{1}{3},Nc_0 \end{pmatrix}$$

These rhombohedral axes can of course be described in terms of threefold primitive hexagonal axes with $c=3Nc_0$. In these axes the plus sign corresponds to the obverse setting and the minus sign to the reverse for the rhombohedral axes (Vol. I, 2.5).

The symmetry of the possible packing arrangements of close-packed planes is exhibited for $N \leq 12$ in Table 7.1.5B, which is a modification and amplification of that of Zhdanov [17]. A detailed description of this table precedes it.

TABLE 7.1.5B

Symmetry of Stacked Closest-packed Layers

Description

This table exhibits and classifies the closest-packed structures for which the period N is less than or equal to 12. It is best described and explained in terms of the methods which have been used in its construction and which may be used in its extension.

Partitions

The period N is first partitioned in all possible ways of order two. One of the numbers of each partition will correspond to positive changes between layers in the Zhdanov notation, while the other will correspond to negative changes. For example, for $N=8$ the second-order partitions are 71,62,53,44. The lattice type for each partition is then determined (e.g. 71,44 are hexagonal, 62,53 are rhombohedral). Each of the two terms is then partitioned in all possible ways and the partitions which are of the same order are interleaved in all the possible ways which give different Zhdanov symbols. Thus in 53, the partitions of 5 are 41,32,311,221; while those of 3 are 21,111 and the possible symbols are 4211,3221 and 31111,21211, where the partitions of 5 which are of one sign are here underlined to distinguish them from the partitions of 3 which are of opposite sign. Also in 44, the partitions of 4 are 31,22,211,1111 and the symbols of interest are 3113,3212,221111,211211. The symbols 2222 and 1111111 are discarded as belonging to $N=4$ and $N=2$ respectively. In this way all possible cases for a given N can be exhibited.

Symmetry Properties

The lowest symmetries which can be exhibited by periodic stacking of closest-packed layers are $P3m$ and $R3m$. Higher symmetries than these result from the satisfaction of one or more of the following

conditions in the partitions of sign changes obtained from the above routine.

$\bar{1}$ A symmetry centre appears in the Zhdanov notation as a symmetrical arrangement of the numbers of *like* signs surrounding a single number. Thus in (4)231(3)132, the sign successions (4) and (3) enclosed in parentheses each contain centres of symmetry. Note that such parentheses contain a *single* succession number and that (11) in the tables means a sequence of eleven signs and *not* two sequences of one sign. If the centrosymmetrical succession is even, the centre lies in a *sphere*. If it is odd, the centre lies in an *octahedral void*. Three cases arise and are used in classification:

$\bar{1}(S)$: Both centro-successions even and both centres in spheres, e.g. (4)3(2)3.

$\bar{1}(O)$: Both centro-successions odd and both centres in octahedral voids, e.g. (3)2(1)2.

$\bar{1}(SO)$: One succession even and one odd, and one centre of each type, e.g. (4)2(1)2.

In the tables parentheses enclose sequence numbers which contain centres.

m A symmetry plane appears as a symmetrical arrangement of the numbers of *opposite* signs grouped about the space between two succession numbers, e.g. |311|113|. Here and in the tables a vertical line is used to indicate a plane of symmetry which can occur only *within* a close-packed layer of spheres.

6_3 The screw axis 6_3 requires that the first half-period of the sequence contains an odd number of succession numbers which is repeated identically (but corresponding to opposite signs) in the second half-period, e.g. 123123, which is the only sequence with this symmetry in the range of the table.

Combinations of these symmetry elements with the symmetry properties of the close-packed plane and with those of the lattices P and R give rise to seven space-group symmetries: $P3m1$; $P\bar{3}m1$ (S,O,SO); $P\bar{6}m2$; $P6_3mc$; $P6_3/mmc$ (S,O); $R3m$; $R\bar{3}m$ (S,O,SO).

For convenience of presentation the table is divided into five parts. This division, which is quite arbitrary, is summarized below.

Part	N	Basic Partition	Lattice	Space Groups
A.	Even	Like	P	$P6_3/mmc(S,O)$; $P6_3mc$; $P\bar{6}m2$; $P\bar{3}m1(S,O)$; $P3m1$
B.	Even	Unlike	P	$P\bar{3}m1(S,O)$; $P3m1$
C.	Even	Unlike	R	$R\bar{3}m(S,O)$; $R3m$
D.	Odd	Unlike	P	$P\bar{3}m1(SO)$; $P3m1$
E.	Odd	Unlike	R	$R\bar{3}m(SO)$; $R3m$

Detailed tables of the co-ordinates for the closest-packed arrangements are beyond the scope of the present publication. A method which may be used in deriving such tables can be learned from the following examples (see previous column) for explanation of symbols (S), (O), (SO).

EXAMPLE 1. Space group $P3m1$: Symbol 4221: $N=9$.

Starting with an A layer and positive signs, the symbol is translated as follows:

	+	+	+	+	-	-	+	+	-
A	B	C	A	B	A	C	A	B	A
0	1	2	3	4	5	6	7	8	0

The A-layers are then in the special positions $1(a):0,0,z$ of $P3m1$ with $z=0, \frac{3}{9}, \frac{5}{9}, \frac{7}{9}$; the B-layers in $1(c): \frac{2}{3}, \frac{1}{3}, z$ with $z=\frac{1}{9}, \frac{4}{9}, \frac{8}{9}$; and the C-layers in $1(b): \frac{1}{3}, \frac{2}{3}, z$ with $z=\frac{2}{9}, \frac{6}{9}$.

EXAMPLE 2. Space group $R3m$: symbol 4211: $N=8$.

In the rhombohedral lattices it is convenient to work in the threefold centred hexagonal cell of period $3N$. It is also convenient to allocate the signs to the symbol so that $p-n \equiv -1 \pmod{3}$ in which case a B-layer in the first period becomes an A-layer in the second period, while a C-layer in the first period becomes an A-layer in the third period. We may thus record the co-ordinates of all layers as A layers, the corresponding B and C layers being located as the space-group equivalents of the A layers. The symbol in the present case satisfies these conditions if we start with positive signs, i.e. $(4+1)-(2+1)=2 \equiv -1 \pmod{3}$. We thus make the translation

	+	+	+	+	-	-	+	-
A	B	C	A	B	A	C	A	[C]
0	1	2	3	4	5	6	7	0

in which only the layers of the first period are shown with the exception of [C], which indicates the start of the second. The co-ordinates are thus $R3m:1(a):0,0,z$ in the hexagonal notation with $z=0, \frac{3}{24}, \frac{5}{24}, \frac{7}{24}; (1+8)/24; (4+8)/24; (2+16)/24; (6+16)/24$, i.e. the co-ordinates are 0,3,5,7,9,12,18,22 all expressed in 24ths.

EXAMPLE 3. Space group $P\bar{3}m1(S)$: symbol (4)3(2)3: $N=12$.

NOTE. The procedure of this example applies with obvious modifications to the space groups $P6_3/mmc(S)$; $P\bar{3}m1(SO)$; $R\bar{3}m(S)$; $R\bar{3}m(SO)$.

	+	+	-	-	-	+	+	-	-	-	+	+
(A)	B	C	B	A	C	(A)	B	A	C	B	C	(A)
0	1	2	3	4	5	6	7	8	9	10	11	12

Note now that in this space group as set up in the tables the C-layer provides the type position for $2(d): \frac{1}{3}, \frac{2}{3}, z; \frac{2}{3}, \frac{1}{3}, \bar{z}$. Thus the positions occupied are $1(a): 0,0,0; 1(b): 0,0,\frac{1}{2}; 2(c): 0,0,z; 0,0,\bar{z}$, with $z=\frac{4}{12}$; and $2(d): \frac{1}{3}, \frac{2}{3}, z; \frac{2}{3}, \frac{1}{3}, \bar{z}$ with $z=\frac{2}{12}, \frac{5}{12}, \frac{9}{12}, \frac{11}{12}$.

7.1. CLOSE PACKING

TABLE 7.1.5B (continued)

Symmetry of Stacked Closest-packed Layers

A. Period Even; Basic Partitions Like; Hexagonal Lattice

<i>N</i>	<i>P6₃mmc</i>		<i>P6₃mc</i>	<i>P6̄m2</i>	<i>P3̄m1</i>		<i>P3m1</i>	Cases
	<i>S</i>	<i>O</i>			<i>S</i>	<i>O</i>		
2		(1) (1)						1
4	(2) (2)							1
6		(3) (3)		21 12				2
8	(4) (4) ; 1(2)1 1(2)1			31 13 ; 211 112		(3)2(1)2		5
10		(5) (5) ; 1(3)1 1(3)1 ; 2(1)2 2(1)2		41 14 ; 32 23 ; 311 113 ; 221 122 ; 2111 1112 ; 1211 1121		(3)21(1)12	4312; 321211	12
12	(6) (6) ; 1(4)1 1(4)1 ; 11(2)11 11(2)11		123123	51 15 ; 42 24 ; 411 114 ; 123 321 ; 231 132 ; 312 213 ; 2211 1122 ; 2121 1212 ; 3111 1113 ; 1311 1131 ; 21111 11112 ; 12111 11121	(4)3(2)3; (4)21(2)12; (2)211(2)112	(5)3(1)3; (1)221(1)122; (3)211(1)112; (3)112(1)211	5412; 342111; 312411; 312114; 332211; 322212; 32121111; 32111211	31

TABLE 7.1.5B (continued)

B. Period Even; Basic Partitions Unlike; Hexagonal Lattice

<i>N</i>	Basic Partitions	<i>P3̄m1</i>		<i>P3m1</i>	Cases
		<i>S</i>	<i>O</i>		
8	7 1		(7)(1)		1
10	8 2	(8)(2) (6)1(2)1	(7)1(1)1; (5)1(3)1		4
12	9 3		(9)(3); (7)11(1)11; (5)12(1)21; (1)14(1)41	8211; 7221; 6231; 5241 612111; 513111; 413121	11

7.1. CLOSE PACKING

TABLE 7.1.5B (continued)

C. Period Even; Basic Partition Unlike; Rhombohedral Lattice

N	Basic Partition	$R\bar{3}m$		$R3m$	Cases	
		S	O			
4	3 1		(3)(1)		1	1
6	5 1 4 2	(4)(2)	(5)(1) (3)1(1)1		1 2	3
8	6 2 5 3	(6)(2); (4)1(2)1	(5)1(1)1 (5)(3); (3)11(1)11; (1)21(1)12	4211; 3221	3 5	8
10	9 1 7 3 6 4	(6)(4); (4)2(2)2; (4)11(2)11; (2)21(2)12	(9)(1) (7)(3); (5)11(1)11; (3)12(1)21; (1)31(1)13 (5)2(1)2; (3)3(1)3; (3)111(1)111; (1)211(1)112	6211; 5221; 4231; 412111 5311; 4321; 421111; 322111; 321121; 312211	1 8 14	23
12	11 1 10 2 8 4 7 5	(10)(2); (8)1(2)1; (6)1(4)1 6 cases omitted	(11)(1) (9)1(1)1; (7)1(3)1 6 cases omitted 10 cases omitted	 14 cases omitted 28 cases omitted	1 5 26 38	70

NOTE. (10) and (11) in these tables refer to the single succession numbers ten and eleven.

TABLE 7.1.5B (continued)

D. Period Odd; Hexagonal Lattice

N	Basic Partition	$P\bar{3}m1(SO)$	$P3m1$	Cases	
5	4 1	(4)(1)		1	
7	5 2	(5)(2); (4)1(1)1; (3)1(2)1		3	
9	6 3	(6)(3); (2)3(1)3; (4)11(1)11	5211; 4221; 312111	6	
11	10 1 7 4	(10)(1) (7)(4); (6)2(1)2; (5)2(2)2; (4)2(3)2; (5)11(2)11; (3)12(2)21; (2)31(1)13; (4)111(1)111; (3)111(2)111; (2)121(1)121	6311; 5321; 4331; 521111; 422111; 421121; 412211; 313211; 322121; 31211111	1 20	21

TABLE 7.1.5B (*continued*)
E. Period Odd; Rhombohedral Lattice

<i>N</i>	Basic Partition	$R\bar{3}m(SO)$	$R3m$	Cases	
1	1 0	(1)(0)		1	
3	2 1	(2)(1)		1	
5	3 2	(3)(2); (2)1(1)1		2	
7	6 1 4 3	(6)(1) (4)(3); (2)2(1)2; (2)11(1)11	3211	1 4	5
9	8 1 7 2 5 4	(8)(1) (7)(2); (6)1(1)1; (5)1(2)1; (4)1(3)1 (5)(4); (4)2(1)2; (3)2(2)2; (3)11(2)11; (2)21(1)12; (2)111(1)111	4311; 3321; 321111; 221211	1 4 10	15
11	9 2 8 3 6 5	(9)(2); (8)1(1)1; (7)1(2)1; (6)1(3)1; (5)1(4)1 (8)(3); (2)4(1)4; (6)11(1)11; (4)12(1)21; (2)13(1)31 10 cases omitted	7211; 6221; 5231; 512111; 413111 16 cases omitted	5 10 26	41

EXAMPLE 4. Space group $P\bar{3}m1(O)$: symbol (3)2(1)2; $N=8$.

NOTE. The procedure of this example applies with obvious modifications to the space groups $P6_3/mmc(O)$; $R\bar{3}m(O)$.

(+) + - - (+) - - + (+)
 C A C B C B A B
 1 3 5 7 9 11 13 15

In this case the z co-ordinates are odd numbers of $2N$ ths of the period, since the centre at the origin is midway between two layers. Note also that a B-layer must be taken below and a C-layer above if the sign at the origin is +. This is to ensure that the void is in an A-position. For the present case the positions are $2(c)$: $0,0,z$; $0,0,\bar{z}$ with $z=\frac{3}{16}$ and $2(d)$: $\frac{1}{3},\frac{2}{3},z$; $\frac{2}{3},\frac{1}{3},\bar{z}$ with $z=\frac{1}{16},\frac{5}{16},\frac{9}{16}$.

EXAMPLE 5. Space Group $P\bar{6}m2$: Symbol $|31|13|$: $N=8$.

| + + + - | + - - - |
 A B C A C A C B A
 0 1 2 3 4 5 6 7 0

The occupied positions are clearly $1(a)$: $0,0,0$; $1(d)$: $\frac{1}{3},\frac{2}{3},\frac{1}{2}$; $2(g)$: $0,0,z$; $0,0,\bar{z}$ with $z=\frac{3}{8}$; $2(h)$: $\frac{1}{3},\frac{2}{3},z$; $\frac{1}{3},\frac{2}{3},\bar{z}$ with $z=\frac{2}{8}$; $2(i)$: $\frac{2}{3},\frac{1}{3},z$; $\frac{2}{3},\frac{1}{3},\bar{z}$ with $z=\frac{1}{8}$.

EXAMPLE 6. Space Group $P6_3mc$: Symbol 123123: $N=12$.

+ - - + + + - + + - - -
 C A C B C A B A B C B A [C]
 0 1 2 3 4 5 6 7 8 9 10 11 0
(Setting I)

The allocation of letter symbols in sequences of this type is governed, in accordance with the setting of the space group (Vol. I), by the following rules concerning the signs in the *first half-period*:

1. If $p-n \equiv 0 \pmod{3}$, the first and second half-periods both start with A-positions, and there is a sphere at the origin.
2. If $p-n \equiv 1 \pmod{3}$, the first sequence must start with B and the second with C (B \rightarrow C: +), and the origin is in an octahedral void.
3. If $p-n \equiv -1 \pmod{3}$, the first sequence must start with C and the second with B (C \rightarrow B: -), and the origin is in an octahedral void.

Setting I above obeys Rule 3, and C is therefore chosen for $z=0$. The co-ordinates are then $2(a)$: $0,0,z$, $0,0,\frac{1}{2}+z$ with $z=1,5$; $2(b)$: $\frac{1}{3},\frac{2}{3},z$; $\frac{2}{3},\frac{1}{3},\frac{1}{2}+z$ with $z=0,2,4,9$ (twelfths).

As an alternative we could write the symbol 231231 and obtain the arrangement (Rule 1)

+ + - - - + - - + + + -
 A B C B A C A C B C A B [A]
 0 1 2 3 4 5 6 7 8 9 10 11 0
(Setting II)

Co-ordinates: $2(a)$ with $z=0,4$; $2(b)$ with $z=2,5,7,9$ (twelfths).

It is also permissible to split a sequence of signs to permit a sphere to be located at the origin, e.g.

+ - + + - - - + - - + +
 A B A B C B A C A C B C [A]
 0 1 2 3 4 5 6 7 8 9 10 11 0
(Setting III)

Co-ordinates: 2(a) with $z=0,2$; 2(b) with $z=4,7,9,11$ (twelfths). This procedure would be necessary to locate a sphere at the origin in 136136, since there is no rearrangement that will satisfy Rule 1.

7.1.6. Structures related to Closest Packing

In many crystals a "closest-packed" arrangement of ionized atoms (not necessarily in contact) occurs in which some of the interstices are filled with smaller ions. Notable examples are to be found among the alkali halides and the spinels; and many other examples are given in the literature.

In many covalent structures of the AB type in which the co-ordination is tetrahedral an atom A lies in the tetrahedral voids of a closest-packed arrangement of the B atoms (although the latter are again not of course in "contact"). An example is provided by the modifications of SiC. In these structures all the types of closest-packed arrangements referred to in the preceding section can occur, although the sequence of numbers seems to be limited to 2,3,4 by the physical chemistry of the system (cf. Ramsdell and Kohn [15]). In structures of this type any one of the space-group symmetries mentioned above may be exhibited in the arrangement of one type of atom *taken alone*. The full symmetry is, however, lowered by the presence of the second atom, and the structures of this type are limited to the space groups $P6_3mc$, $P3m1$ and $R3m$, which have neither horizontal planes of symmetry nor centres.

Similar generalizations are theoretically possible for the diamond structure and for the tetrahedral rarest packing referred to in Table 7.1.3.

7.1.7. Radial Distribution of Atoms

(a) Cubic Structures

With a spherical atom of *diameter* unity centred at the origin, the Cartesian co-ordinates of other atoms and the formulae for their distances (R) are as shown in Table 7.1.7A.

The distances, co-ordinates, and multiplicities of successive neighbours ($R \leq 6$) are given in Tables 7.1.7B, C, D. The construction and extension of these tables is aided by the use of tables of the cubic quadratic form (Table 3.8.6A, p. 124) and of multiplicities for the cubic system (Vol. I, Table 3.5.1). Tables 7.1.7B, C, D also list the number of spheres contained in or on a sphere of radius R .

(b) Hexagonal Closest Packing

With a sphere of *diameter* unity centred at the origin the Cartesian co-ordinates of the atoms are of two types: (1) $p, q, (\sqrt{\frac{2}{3}})r$ and (2) $(3p-1)/3, (3q-2)/3, (\sqrt{\frac{2}{3}})r$, where p, q, r are positive or negative integers or zero. Co-ordinates (1) are applicable for r even and co-ordinates (2) for r odd. The corresponding distances are given by

$$R_1^2 = p^2 + q^2 - pq + \frac{2}{3}r^2$$

$$R_2^2 = \left[\left(\frac{3p-1}{3} \right)^2 + \left(\frac{3q-2}{3} \right)^2 - \left(\frac{3p-1}{3} \right) \left(\frac{3q-2}{3} \right) \right] + \frac{2}{3}r^2$$

$$= p^2 + q^2 - pq - q + \frac{1}{3} + \frac{2}{3}r^2$$

Table 7.1.7E lists the distances and multiplicities for successive neighbours to $R \leq 6$ and the total number of spheres in or on a sphere of radius R .

TABLE 7.1.7A

Radial Distribution of Atoms in the Three Cubic Lattices

A spherical atom, diameter unity, is centred at the origin. The table gives Cartesian co-ordinates and distances R of atoms at lattice points pqr .

| Structure type | Cartesian co-ordinates | R^2 | Remarks |
|------------------------------|--|--------------------------------------|--------------------------------|
| Simple cubic | p, q, r | $R^2 = p^2 + q^2 + r^2$ | All values of p, q, r . |
| Body-centred cubic | $\frac{p}{\sqrt{3}}, \frac{q}{\sqrt{3}}, \frac{r}{\sqrt{3}}$ | $R^2 = \frac{1}{3}(p^2 + q^2 + r^2)$ | p, q, r all even or all odd. |
| Face-centred cubic | $\frac{p}{\sqrt{2}}, \frac{q}{\sqrt{2}}, \frac{r}{\sqrt{2}}$ | $R^2 = \frac{1}{2}(p^2 + q^2 + r^2)$ | $p+q+r=2n$ |

For all cases p, q, r are positive or negative integers or zero.

7.1. CLOSE PACKING

TABLE 7.1.7B

Simple Cubic

| pqr | R | R^2 | M | Total |
|------------------|--------|-------|-----|-------|
| 000 | 0 | 0 | 1 | |
| 100 | 1.0000 | 1 | 6 | 7 |
| 110 | 1.4142 | 2 | 12 | 19 |
| 111 | 1.7321 | 3 | 8 | 27 |
| 200 | 2.0000 | 4 | 6 | 33 |
| 210 | 2.2361 | 5 | 24 | 57 |
| 211 | 2.4495 | 6 | 24 | 81 |
| 220 | 2.8284 | 8 | 12 | 93 |
| 300(6), 221(24) | 3.0000 | 9 | 30 | 123 |
| 310 | 3.1623 | 10 | 24 | 147 |
| 311 | 3.3166 | 11 | 24 | 171 |
| 222 | 3.4641 | 12 | 8 | 179 |
| 320 | 3.6056 | 13 | 24 | 203 |
| 321 | 3.7417 | 14 | 48 | 251 |
| 400 | 4.0000 | 16 | 6 | 257 |
| 410(24), 322(24) | 4.1231 | 17 | 48 | 305 |
| 411(24), 330(12) | 4.2426 | 18 | 36 | 341 |
| 331 | 4.3589 | 19 | 24 | 365 |
| 420 | 4.4721 | 20 | 24 | 389 |
| 421 | 4.5826 | 21 | 48 | 437 |
| 332 | 4.6904 | 22 | 24 | 461 |
| 422 | 4.8990 | 24 | 24 | 485 |
| 500(6), 430(24) | 5.0000 | 25 | 30 | 515 |
| 510(24), 431(48) | 5.0990 | 26 | 72 | 587 |
| 511(24), 333(8) | 5.1962 | 27 | 32 | 619 |
| 520(24), 432(48) | 5.3852 | 29 | 72 | 691 |
| 521 | 5.4772 | 30 | 48 | 739 |
| 440 | 5.6569 | 32 | 12 | 751 |
| 522(24), 441(24) | 5.7446 | 33 | 48 | 799 |
| 530(24), 433(24) | 5.8310 | 34 | 48 | 847 |
| 531 | 5.9161 | 35 | 48 | 895 |
| 600(6), 442(24) | 6.0000 | 36 | 30 | 925 |

7.1. CLOSE PACKING

TABLE 7.1.7C
Body-centred Cubic

| pqr | R | R^2 | M | Total |
|---------------------------|--------|-------|-----|-------|
| 000 | 0 | 0 | 1 | |
| 111 | 1.0000 | 1 | 8 | 9 |
| 200 | 1.1547 | 4/3 | 6 | 15 |
| 220 | 1.6330 | 8/3 | 12 | 27 |
| 311 | 1.9149 | 11/3 | 24 | 51 |
| 222 | 2.0000 | 4 | 8 | 59 |
| 400 | 2.3094 | 16/3 | 6 | 65 |
| 331 | 2.5166 | 19/3 | 24 | 89 |
| 420 | 2.5820 | 20/3 | 24 | 113 |
| 422 | 2.8284 | 8 | 24 | 137 |
| 511(24), 333(8) | 3.0000 | 9 | 32 | 169 |
| 440 | 3.2660 | 32/3 | 12 | 181 |
| 531 | 3.4157 | 35/3 | 48 | 229 |
| 600(6), 442(24) | 3.4641 | 12 | 30 | 259 |
| 620 | 3.6515 | 40/3 | 24 | 283 |
| 533 | 3.7859 | 43/3 | 24 | 307 |
| 622 | 3.8297 | 44/3 | 24 | 331 |
| 444 | 4.0000 | 16 | 8 | 339 |
| 711(24), 551(24) | 4.1231 | 17 | 48 | 387 |
| 640 | 4.1633 | 52/3 | 24 | 411 |
| 642 | 4.3205 | 56/3 | 48 | 459 |
| 731(48), 553(24) | 4.4347 | 59/3 | 72 | 531 |
| 800 | 4.6188 | 64/3 | 6 | 537 |
| 733 | 4.7258 | 67/3 | 24 | 561 |
| 820(24), 644(24) | 4.7610 | 68/3 | 48 | 609 |
| 822(24), 660(12) | 4.8990 | 24 | 36 | 645 |
| 751(48), 555(8) | 5.0000 | 25 | 56 | 701 |
| 662 | 5.0332 | 76/3 | 24 | 725 |
| 840 | 5.1640 | 80/3 | 24 | 749 |
| 911(24), 753(48) | 5.2599 | 83/3 | 72 | 821 |
| 842 | 5.2915 | 28 | 48 | 869 |
| 664 | 5.4160 | 88/3 | 24 | 893 |
| 931 | 5.5076 | 91/3 | 48 | 941 |
| 844 | 5.6569 | 32 | 24 | 965 |
| 933(24), 771(24), 755(24) | 5.7446 | 33 | 72 | 1037 |
| 10,0,0(6); 860(24) | 5.7735 | 100/3 | 30 | 1067 |
| 10,2,0(24), 862(48) | 5.8878 | 104/3 | 72 | 1139 |
| 951(48), 773(24) | 5.9722 | 107/3 | 72 | 1211 |
| 10,2,2(24), 666(8) | 6.0000 | 36 | 32 | 1243 |

7.1. CLOSE PACKING

TABLE 7.1.7D
Face-centred Cubic

| pqr | R | R^2 | M | Total |
|---------------------------|--------|-------|-----|-------|
| 000 | 0 | 0 | 1 | |
| 110 | 1.0000 | 1 | 12 | 13 |
| 200 | 1.4142 | 2 | 6 | 19 |
| 211 | 1.7321 | 3 | 24 | 43 |
| 220 | 2.0000 | 4 | 12 | 55 |
| 310 | 2.2361 | 5 | 24 | 79 |
| 222 | 2.4495 | 6 | 8 | 87 |
| 321 | 2.6458 | 7 | 48 | 135 |
| 400 | 2.8284 | 8 | 6 | 141 |
| 411(24), 330(12) | 3.0000 | 9 | 36 | 177 |
| 420 | 3.1623 | 10 | 24 | 201 |
| 332 | 3.3166 | 11 | 24 | 225 |
| 422 | 3.4641 | 12 | 24 | 249 |
| 510(24), 431(48) | 3.6056 | 13 | 72 | 321 |
| 521 | 3.8730 | 15 | 48 | 369 |
| 440 | 4.0000 | 16 | 12 | 381 |
| 530(24), 433(24) | 4.1231 | 17 | 48 | 429 |
| 600(6), 442(24) | 4.2426 | 18 | 30 | 459 |
| 611(24), 532(48) | 4.3589 | 19 | 72 | 531 |
| 620 | 4.4721 | 20 | 24 | 555 |
| 541 | 4.5826 | 21 | 48 | 603 |
| 622 | 4.6904 | 22 | 24 | 627 |
| 631 | 4.7958 | 23 | 48 | 675 |
| 444 | 4.8990 | 24 | 8 | 683 |
| 710(24), 550(12), 543(48) | 5.0000 | 25 | 84 | 767 |
| 640 | 5.0990 | 26 | 24 | 791 |
| 721(48), 633(24), 552(24) | 5.1962 | 27 | 96 | 887 |
| 642 | 5.2915 | 28 | 48 | 935 |
| 730 | 5.3852 | 29 | 24 | 959 |
| 732(48), 651(48) | 5.5678 | 31 | 96 | 1055 |
| 800 | 5.6569 | 32 | 6 | 1061 |
| 811(24), 741(48), 554(24) | 5.7446 | 33 | 96 | 1157 |
| 820(24), 644(24) | 5.8310 | 34 | 48 | 1205 |
| 653 | 5.9161 | 35 | 48 | 1253 |
| 822(24), 660(12) | 6.0000 | 36 | 36 | 1289 |

7.1. CLOSE PACKING

TABLE 7.1.7E
Hexagonal Closest Packing

| R | R^2 | M | Total | R | R^2 | M | Total |
|--------|-------|-----|-------|--------|-------|-----|-------|
| 0 | 0 | 1 | | 4.2817 | 55/3 | 12 | 479 |
| 1.0000 | 1 | 12 | 13 | 4.3205 | 56/3 | 12 | 491 |
| 1.4142 | 2 | 6 | 19 | 4.3589 | 19 | 24 | 515 |
| 1.6330 | 8/3 | 2 | 21 | 4.4347 | 59/3 | 12 | 527 |
| 1.7321 | 3 | 18 | 39 | 4.5092 | 61/3 | 12 | 539 |
| 1.9149 | 11/3 | 12 | 51 | 4.5826 | 21 | 36 | 575 |
| 2.0000 | 4 | 6 | 57 | 4.6547 | 65/3 | 24 | 599 |
| 2.2361 | 5 | 12 | 69 | 4.6904 | 22 | 12 | 611 |
| 2.3805 | 17/3 | 12 | 81 | 4.7258 | 67/3 | 18 | 629 |
| 2.4495 | 6 | 6 | 87 | 4.7610 | 68/3 | 12 | 641 |
| 2.5166 | 19/3 | 6 | 93 | 4.7958 | 23 | 24 | 665 |
| 2.5820 | 20/3 | 12 | 105 | 4.8305 | 70/3 | 12 | 677 |
| 2.6458 | 7 | 24 | 129 | 4.8648 | 71/3 | 48 | 725 |
| 2.7080 | 22/3 | 6 | 135 | 4.8990 | 24 | 2 | 727 |
| 2.8868 | 25/3 | 12 | 147 | 5.0000 | 25 | 36 | 763 |
| 3.0000 | 9 | 12 | 159 | 5.0990 | 26 | 24 | 787 |
| 3.1091 | 29/3 | 24 | 183 | 5.1316 | 79/3 | 12 | 799 |
| 3.1623 | 10 | 12 | 195 | 5.1640 | 80/3 | 12 | 811 |
| 3.2146 | 31/3 | 12 | 207 | 5.1962 | 27 | 42 | 853 |
| 3.2660 | 32/3 | 2 | 209 | 5.2281 | 82/3 | 6 | 859 |
| 3.3166 | 11 | 12 | 221 | 5.2599 | 83/3 | 12 | 871 |
| 3.3665 | 34/3 | 6 | 227 | 5.2915 | 28 | 24 | 895 |
| 3.4157 | 35/3 | 24 | 251 | 5.3229 | 85/3 | 12 | 907 |
| 3.4641 | 12 | 6 | 257 | 5.3852 | 29 | 12 | 919 |
| 3.5119 | 37/3 | 12 | 269 | 5.4467 | 89/3 | 36 | 955 |
| 3.6056 | 13 | 24 | 293 | 5.5076 | 91/3 | 12 | 967 |
| 3.6968 | 41/3 | 12 | 305 | 5.5377 | 92/3 | 24 | 991 |
| 3.7859 | 43/3 | 6 | 311 | 5.5678 | 31 | 72 | 1063 |
| 3.8297 | 44/3 | 24 | 335 | 5.5976 | 94/3 | 12 | 1075 |
| 3.8730 | 15 | 12 | 347 | 5.6273 | 95/3 | 24 | 1099 |
| 3.9158 | 46/3 | 12 | 359 | 5.6862 | 97/3 | 12 | 1111 |
| 3.9581 | 47/3 | 24 | 383 | 5.7446 | 33 | 48 | 1159 |
| 4.0000 | 16 | 6 | 389 | 5.8023 | 101/3 | 24 | 1183 |
| 4.0415 | 49/3 | 12 | 401 | 5.8310 | 34 | 24 | 1207 |
| 4.1231 | 17 | 24 | 425 | 5.9161 | 35 | 24 | 1231 |
| 4.2032 | 53/3 | 24 | 449 | 5.9722 | 107/3 | 12 | 1243 |
| 4.2426 | 18 | 18 | 467 | 6.0000 | 36 | 18 | 1261 |

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7.2. The Use of Statistical Methods for the Detection of Symmetry Elements

By V. LUZZATI

Notation

\mathbf{s} = position vector in reciprocal space
($s=\{2 \sin \theta\}/\lambda$).

$\Phi(\mathbf{s}) = \sum_{j=1}^N f_j^2(\mathbf{s})$, where $f_j(\mathbf{s})$ is the scattering factor
of the j atom and N is the number of
atoms contained in the unit cell.

$I(\mathbf{s})$ = observed intensity corrected to give F^2 at the
end-point of \mathbf{s} .

$\langle I(\mathbf{s}) \rangle$ = average value of $I(\mathbf{s})$ for all the points of the
reciprocal lattice contained within a thin
spherical shell of radius s .

$P(I)dI$ = fraction of the reciprocal lattice points
where the intensity lies between I and
 $I+dI$.

S = distribution parameter [9] [14].

Validity of Statistical Methods

The rigorous and general validity of the methods
described below has been proved only when the
statistical analysis is performed using all the points of
the reciprocal space. Nevertheless, in practical appli-
cations, only a limited volume of the reciprocal space
is accessible; in this case the validity is subject to some
restrictions: (a) the number of the crystallographically
independent atoms must be large, (b) no atom must
be predominant, (c) the distribution of atomic posi-
tions in the unit cell must be random. These restric-
tions are the more severe the nearer the reciprocal
lattice points used in the statistical analysis are to the
origin [1] [2] [4] [7] [12].

7.2.1. Determination of the Absolute Scale and of the Thermal Vibration Factor

It has been shown that

$$\langle I(\mathbf{s}) \rangle = \alpha \Phi(\mathbf{s}) \quad \dots (1)$$

(see references [1] [5] [12] [14]).

Equation (1) is valid for general reflections con-
tained in the three-dimensional reciprocal lattice (hkl),
as well as for zones and rows containing the origin (say
 $hk0$ or $h00$); α is an integral factor whose value depends
upon the class of reflections (that is, hkl , or $hk0$, or
 $h00$) and the symmetry elements of the unit cell. The
values of α are given in Tables 7.2.1A and 7.2.1B: the
average $\langle I \rangle$ always refers to all the reflections, even
in the cases when a fraction of the reflections are
systematically absent [14].

If the chemical composition of the unit cell is known,
and if the atoms are subject to an isotropic thermal

vibration (the same amplitude for all the atoms),
equation (1) can be used to determine the absolute
scale and the thermal vibration factor, which affect the
experimental intensities.

TABLE 7.2.1A

Intensity-distribution Effects of Symmetry Elements
not causing Systematic Absences

(C=centrosymmetric distribution; A=non-centrosym-
metric distribution; Z=systematically zero. Axes are
parallel to \mathbf{c} , planes perpendicular to \mathbf{c} .)

| Symmetry
element | Reflections | Distribution | $\alpha=S/\Phi$
$=\langle I \rangle/\Phi$ |
|---------------------|-------------|--------------|--|
| 1 | all | A | 1 |
| $\bar{1}$ | all | C | 1 |
| 2 | hkl | A | 1 |
| | $hk0$ | C | 1 |
| | $00l$ | A | 2 |
| $\bar{2}=m$ | hkl | A | 1 |
| | $hk0$ | A | 2 |
| | $00l$ | C | 1 |
| 3 | hkl | A | 1 |
| | $hk0$ | A | 1 |
| | $00l$ | A | 3 |
| $\bar{3}$ | hkl | C | 1 |
| | $hk0$ | C | 1 |
| | $00l$ | C | 3 |
| 4 | hkl | A | 1 |
| | $hk0$ | C | 1 |
| | $00l$ | A | 4 |
| $\bar{4}$ | hkl | A | 1 |
| | $hk0$ | C | 1 |
| | $00l$ | C | 2 |
| 6 | hkl | A | 1 |
| | $hk0$ | C | 1 |
| | $00l$ | A | 6 |
| $\bar{6}=3/m$ | hkl | A | 1 |
| | $hk0$ | A | 2 |
| | $00l$ | C | 3 |

TABLE 7.2.1B
Intensity-distribution Effects of Symmetry Elements
causing Systematic Absences

| Symmetry element | Reflections | Distribution | $\alpha = \langle I \rangle / \Phi$ | S/Φ |
|------------------|-----------------|-------------------------------|-------------------------------------|----------|
| 2_1 | hkl | A | 1 | 1 |
| | $hk0$ | C | 1 | 1 |
| | $00l$ | $\frac{1}{2}Z + \frac{1}{2}A$ | 1 | 2 |
| $3_1, 3_2$ | hkl | A | 1 | 1 |
| | $hk0$ | A | 1 | 1 |
| | $00l$ | $\frac{2}{3}Z + \frac{1}{3}A$ | 1 | 3 |
| $4_1, 4_3$ | hkl | A | 1 | 1 |
| | $hk0$ | C | 1 | 1 |
| | $00l$ | $\frac{3}{4}Z + \frac{1}{4}A$ | 1 | 4 |
| 4_2 | hkl | A | 1 | 1 |
| | $hk0$ | C | 1 | 1 |
| | $00l$ | $\frac{1}{2}Z + \frac{1}{2}A$ | 2 | 4 |
| $6_1, 6_5$ | hkl | A | 1 | 1 |
| | $hk0$ | C | 1 | 1 |
| | $00l$ | $\frac{5}{6}Z + \frac{1}{6}A$ | 1 | 6 |
| $6_2, 6_4$ | hkl | A | 1 | 1 |
| | $hk0$ | C | 1 | 1 |
| | $00l$ | $\frac{2}{3}Z + \frac{1}{3}A$ | 2 | 6 |
| 6_3 | hkl | A | 1 | 1 |
| | $hk0$ | C | 1 | 1 |
| | $00l$ | $\frac{1}{2}Z + \frac{1}{2}A$ | 3 | 6 |
| a | hkl | A | 1 | 1 |
| | $hk0$ | $\frac{1}{2}Z + \frac{1}{2}A$ | 1 | 2 |
| | $00l$ | C | 1 | 1 |
| | $0k0$ | A | 2 | 2 |
| C | hkl | $\frac{1}{2}Z + \frac{1}{2}A$ | 1 | 2 |
| | $hk0, h0l, 0kl$ | $\frac{1}{2}Z + \frac{1}{2}A$ | 1 | 2 |
| | hkh, hkk | $\frac{1}{2}Z + \frac{1}{2}A$ | 1 | 2 |
| | $h0h, 0kk$ | $\frac{1}{2}Z + \frac{1}{2}A$ | 1 | 2 |
| | $h00, 0k0$ | $\frac{1}{2}Z + \frac{1}{2}A$ | 1 | 2 |
| | $hhl, hh0, 00l$ | A | 2 | 2 |
| I | hkl | $\frac{1}{2}Z + \frac{1}{2}A$ | 1 | 2 |
| | $hk0, h0l, 0kl$ | $\frac{1}{2}Z + \frac{1}{2}A$ | 1 | 2 |
| | hhl, hkh, hkk | $\frac{1}{2}Z + \frac{1}{2}A$ | 1 | 2 |
| | $h00, 0k0, 00l$ | $\frac{1}{2}Z + \frac{1}{2}A$ | 1 | 2 |
| | hhh | $\frac{1}{2}Z + \frac{1}{2}A$ | 1 | 2 |
| | $hh0, h0h, 0kk$ | A | 2 | 2 |
| F | hkl | $\frac{3}{4}Z + \frac{1}{4}A$ | 1 | 4 |
| | $hk0, h0l, 0kl$ | $\frac{3}{4}Z + \frac{1}{4}A$ | 1 | 4 |
| | hhl, hkh, hkk | $\frac{1}{2}Z + \frac{1}{2}A$ | 2 | 4 |
| | $hh0, h0h, 0kk$ | $\frac{1}{2}Z + \frac{1}{2}A$ | 2 | 4 |
| | $h00, 0k0, 00l$ | $\frac{1}{2}Z + \frac{1}{2}A$ | 2 | 4 |
| | hhh | A | 4 | 4 |

The relation between the experimental (observed) intensities and the absolute intensities, corrected for the thermal vibration, is

$$I_0(s) = KI_{\text{abs}}(s) \exp\left(-\frac{B}{2}s^2\right) \quad \dots (2)$$

K is the absolute scale factor and B is the parameter that defines the magnitude of the thermal vibration.

Replacing equation (1) in equation (2):

$$\langle I_0(s) \rangle = K\alpha\Phi(s) \exp\left(-\frac{B}{2}s^2\right) \quad \dots (3)$$

A straight line can be obtained by plotting the logarithm of $\langle I_0(s) \rangle / \alpha\Phi(s)$ as a function of s^2 : its extrapolation toward $s=0$ determines the logarithm of K , its slope is $-B/2$.

$$\log \left[\frac{\langle I_0(s) \rangle}{\alpha\Phi(s)} \right] = \log K - \frac{B}{2}s^2 \quad \dots (4)$$

7.2.2. Detection of a Centre of Symmetry

It has been shown that the probability distribution of the intensities is approximately independent of the actual positions of the atoms, and is characteristic of the symmetry of the unit cell.

The distribution laws for all the space groups can be expressed in terms of two fundamental laws, valid respectively for centrosymmetric and non-centrosymmetric cases. If the number of crystallographically independent atoms is large, the distribution laws are [2] [3] [7] [13]:

$${}_1P(I)dI = (2\pi IS)^{-\frac{1}{2}} \exp\left(-\frac{I}{2S}\right) dI \quad \text{(centrosymmetric)} \quad \dots (5)$$

$${}_1P(I)dI = S^{-1} \exp\left(-\frac{I}{S}\right) dI \quad \text{(non-centrosymmetric)} \quad \dots (6)$$

These laws apply to zones and rows, as well as to the whole three-dimensional reciprocal lattice. S is a distribution parameter, proportional to Φ : the ratio S/Φ depends upon the space group and the class of the reflections (that is, hkl , or $hk0$, or $h00$). The values of S/Φ are given in the tables 7.2.1A and 7.2.1B [9] [14].

The difference between the two distribution laws (equations (5) and (6)) can be used to detect the presence of a centre of symmetry, if the experimental intensities are known.

For practical applications it is convenient to normalize the experimental intensities, dividing them by S . A new variable is so defined:

$$z = \frac{I}{S} \quad \dots (7)$$

and the distribution laws become: [4]

$${}_1P(z)dz = (2\pi z)^{-\frac{1}{2}} \exp\left(-\frac{z}{2}\right) dz \quad \dots (8)$$

$${}_1P(z)dz = \exp(-z) dz \quad \dots (9)$$

Several practical tests have been devised. Some of these consist in comparing one parameter, a function of the experimental intensities, with its theoretical

7.2. THE USE OF STATISTICAL METHODS FOR THE DETECTION OF SYMMETRY ELEMENTS

values expected in centrosymmetric and non-centrosymmetric cases. The simplest among the many possible tests of this kind are the average and the variance test.

Average Test [13]

ρ = [(Σ√z) / Σz]^2(10)

The theoretical value of ρ is 2/π (≈0.637) for centrosymmetric, and π/4 (≈0.785) for non-centrosymmetric cases.

Variance Test [15]

V = (Σ(z - z̄)^2) / Σz(11)

The theoretical value of V is 2 for centrosymmetric and 1 for non-centrosymmetric cases.

Other tests consist in the comparison of the distribution law of the experimental intensities, or of some of its moments, with the corresponding theoretical functions.

Zero Moment Test [4]

The fraction N(z) of the reciprocal lattice points where the normalized intensity is smaller than z is:

̄N(z) = erf (½z)† (centrosymmetric)†(12)

₁N(z) = 1 - exp(-z) (non-centrosymmetric)(13)

The functions (12) and (13) are compared in Table 7.2.2 and in the graph (Figure 7.2.2).

In principle all the tests described above are equivalent. Nevertheless the zero moment test is recommended, since it leads to the comparison of two curves instead of only two numbers, and is likely to be less sensitive to the experimental errors.

Since the statistical methods can be used to detect the presence of a centre of symmetry in plane and line projections, as well as in the three-dimensional unit

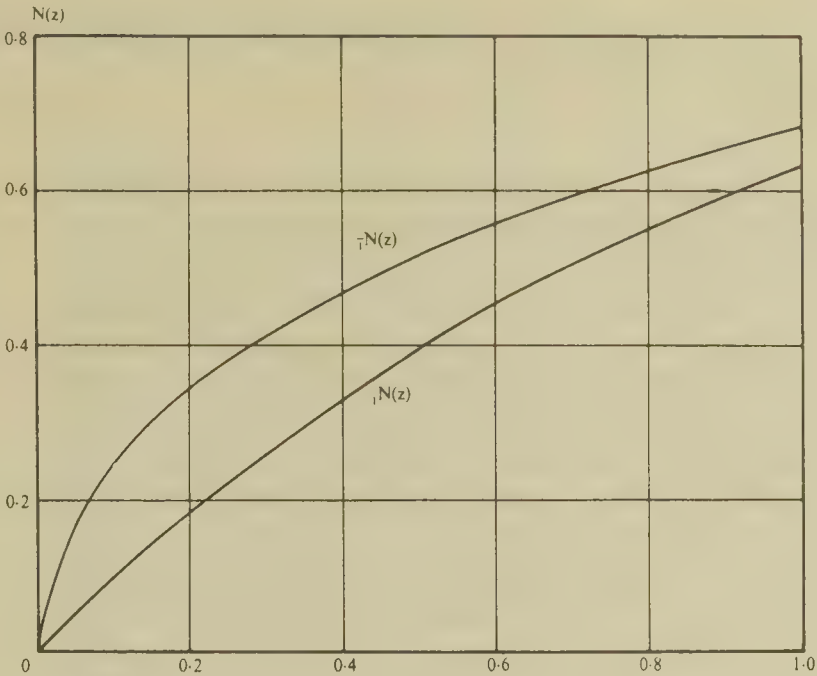


Fig. 7.2.2

cell, they can provide a tool for the determination of some symmetry elements that cannot be detected by the systematic absence of reflections [9] [14].

It has been shown experimentally that the statistical methods in general yield useful information, even when the number of atoms is small. In some cases, when atomic positions are related by some geometrical relationships, in addition to the symmetry operations of the space group (for instance, extra centres of symmetry, or translations), the distribution of intensities can follow special laws [8] [11]. Finally it must be pointed out that experimental errors can have a serious influence upon the distribution laws [10].

† erf(x) is the error function (Jahnke and Emde [6]).

TABLE 7.2.2

Theoretical Values of the Function N(z) for Centrosymmetric and Non-centrosymmetric Cases

| z | 0 | 0.1 | 0.2 | 0.3 | 0.4 | 0.5 | 0.6 | 0.7 | 0.8 | 0.9 | 1.0 |
|-------|---|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| ̄N(z) | 0 | 0.248 | 0.345 | 0.419 | 0.474 | 0.520 | 0.561 | 0.597 | 0.629 | 0.657 | 0.683 |
| ₁N(z) | 0 | 0.095 | 0.181 | 0.259 | 0.330 | 0.393 | 0.451 | 0.503 | 0.551 | 0.593 | 0.632 |

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7.3. Inequality Relations between Structure Factors

By J. BOUMAN

Inequality relations between structure factors in principle provide a means of determining the signs of structure factors for centrosymmetric structures and an indication of the phases for non-centrosymmetric structures. Actually, practical applications of such relations have been made with varying degrees of success in several structure determinations. For a given space group numerous inequalities may be found, but there are no systematic tables for space groups other than $P1$ and $P\bar{1}$, and the problem of the most systematic and economical application is a difficult one to solve. In the present chapter there are given guides on the basis of experience for an efficient procedure in working with inequalities in any space group; also inter-relationships of some simple inequalities, which indicate their relative strengths.

The following considerations are of prime importance:

(a) Relations in which a smaller number of structure factors appear are to be preferred to those with a larger number. Generally, more unknown signs occur in the latter case. Also, in practice, relations containing only the following limited set have been found to be the most useful:

$$F(hkl), F(h'k'l') \quad F(2h, 2k, 2l), F(2h', 2k', 2l') \\ F(h+h', k+k', l+l'), F(h-h', k-k', l-l')$$

(b) Some inequalities may be derived by algebraic means from others, which are then said to be more stringent, since no additional information is to be gained from the derived inequalities. For a given collection of structure factors it is then possible to define a *fundamental set* of inequalities as that set from which all other inequalities may be derived. It is preferable, as a general rule, to work first with the fundamental set.

(c) It may be advisable, nevertheless, to try first a less powerful inequality if it is simpler (i.e. contains fewer structure factors) than a more stringent one.

(d) If possible, the relations between *unitary structure factors* should be used, as these are more powerful than those between the usual structure factors. The unitary structure factor is defined by

$$U(hkl) = \frac{F(hkl)}{Zu}$$

where Z is the total number of electrons in the unit cell, $u = \frac{1}{Z} \sum_{j=1}^N f_j$ is the unitary atomic scattering factor, and $F(hkl)$ is expressed in absolute units. In the following tables only unitary structure factor relations are given. $U(hkl)$ is denoted by U_H ; $U(h+h', k+k', l+l')$ by $U_{H+H'}$; etc.

Table 7.3.1 gives the fundamental set of relations for the structure factors of (a). Some derived inequalities are tabulated in Table 7.3.2 (cf. (c)). Both these tables refer to centrosymmetric structures or projections with a centre of symmetry.

Table 7.3.3 gives the corresponding data for non-centrosymmetric structures. The latter relations are valid for all space groups and those of Tables 7.3.1 and 7.3.2 for all space groups with a centre of symmetry. Inequalities for other symmetry elements are given in Volume I, page 541. The references should be consulted for applications to special space groups.

TABLE 7.3.1

Fundamental Set—Centre of Symmetry ($U_H = U_{-H}$)

1. $2U_H^2 - 1 \leq U_{2H}$
2. $(U_H + U_{H'})^2 \leq (1 + U_{H+H'})(1 + U_{H-H'})$
3. $(U_H - U_{H'})^2 \leq (1 - U_{H+H'})(1 - U_{H-H'})$
4. $(U_{H+H'} - U_{H-H'})^2 \leq (1 - U_{2H})(1 - U_{2H'})$
5. $(U_{H+H'} + U_{H-H'} - 2U_H U_{H'})^2 \leq (1 + U_{2H} - 2U_H^2)(1 + U_{2H'} - 2U_{H'}^2)$

TABLE 7.3.2

Derived Inequalities—Centre of Symmetry

6. $2m|U_H + U_{H'}| \leq 1 + U_{H+H'} + m^2(1 + U_{H-H'})$
7. $2m|U_H - U_{H'}| \leq 1 - U_{H+H'} + m^2(1 - U_{H-H'})$
(m is an arbitrary number)
8. $(U_H + U_{H'})^2 \leq 1 + \frac{1}{2}U_{2H} + \frac{1}{2}U_{2H'} + (U_{H+H'} + U_{H-H'})$
9. $(U_H - U_{H'})^2 \leq 1 + \frac{1}{2}U_{2H} + \frac{1}{2}U_{2H'} - (U_{H+H'} + U_{H-H'})$
10. $(U_{H+H'} + U_{H-H'})^2 \leq (1 + U_{2H})(1 + U_{2H'})$

TABLE 7.3.3

Non-centrosymmetric Structures

Fundamental Set

- 1a. $|U_{H+H'} - U_H U_{H'}|^2 \leq (1 - |U_H|^2)(1 - |U_{H'}|^2)$
- 2a. $|U_{H-H'} - U_H U_{-H'}|^2 \leq (1 - |U_H|^2)(1 - |U_{H'}|^2)$

Derived Inequalities

- 3a. $|U_H + U_{H'}|^2 \leq 2 + U_{H-H'} + U_{H'-H}$
- 4a. $|U_H - U_{H'}|^2 \leq 2 - U_{H-H'} - U_{H'-H}$

It has been shown recently (Bouman, [1]) that all fundamental inequalities for centrosymmetric structures belong to four series. The inequalities belonging to any one series can be arranged in such a way that each inequality contains more structure factors than the preceding ones. The relations 1 and 5 are the first and second inequality of the first series, the relations 4, 2 and 3 are the first inequalities of the second, third and fourth series. It does not seem probable that the higher inequalities will be of practical use.

7.3. INEQUALITY RELATIONS BETWEEN STRUCTURE FACTORS

A fundamental set, as described in Table 7.3.1, is only possible for the structure factors from (a). The n th inequality of the first series and the $(n-1)$ th of the second series contain the same set of structure factors, and they, together with all preceding inequalities, form a fundamental set for these structure factors. The same applies to the n th inequalities of the third and fourth series, but they contain another set of structure factors. Only in the case of Table 7.3.1 can the four series be combined to form one fundamental set.

Numerical and Graphical Examples

Only centrosymmetric structures will be treated here.

Relation 1. If $|U_H| > \frac{1}{2}\sqrt{2} = 0.71$, U_{2H} is positive. If $|U_H| < 0.71$, U_{2H} is positive if its absolute value exceeds $(1 - 2U_H^2)$. If this is not true, nothing can be said about the sign of U_{2H} .

Relations 2 to 10. It is assumed that the signs of U_H and $U_{H'}$ are known and that those of U_{2H} and of $U_{2H'}$ are determined with the help of relation 1. Now the problem of determining the signs of $U_{H+H'}$ and of $U_{H-H'}$ can be elucidated by a graphical representation in the $(U_{H+H'}, U_{H-H'})$ -plane (Fig. 7.3). In this figure the values of the several structure factors are chosen to be $U_H = +0.70$, $U_{H'} = +0.20$, $U_{2H} = +0.29$, $U_{2H'} = +0.32$.

$$|U_{H+H'}| = 0.30, |U_{H-H'}| = 0.25$$

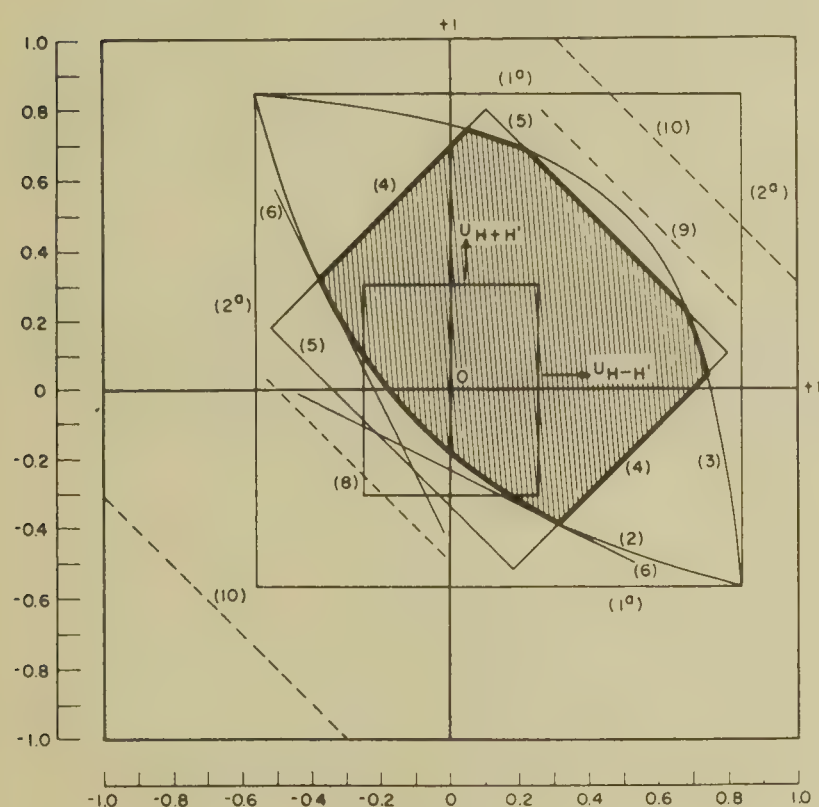


Fig. 7.3

The four possible combinations of signs correspond to four points in the diagram. The inequalities are represented by curves or straight lines, which divide the plane into permitted and forbidden domains. The four inequalities 2, 3, 4, and 5 include the shaded area, which is the permitted domain. It is seen that the combination $U_{H+H'}$ negative, $U_{H-H'}$ negative, is forbidden. Further, the inequalities 6 (with $m = \sqrt{2}$, and $m = \frac{1}{2}\sqrt{2}$) are given. They are tangents to the hyperbola 2. 7 would be represented by a tangent to 3. Also 8, 9, 10, and 1a, 2a, applied to the centrosymmetric structure, are to be found in the diagram. It may be seen from the figure that 6 is derived from 2, 7 from 3, and 8, 9, and 10 from 5. 1a and 2a may be derived from 2 and 3, and also from 4 and 5. In the given example 6 or 8 could be used, too, to get the right answer. The relative situation of the fundamental inequalities is changed if other values of $U_H \dots U_{2H'}$ are chosen (even if the signs only are changed). Thus it cannot be determined beforehand whether all the fundamental inequalities are needed.

Relations 2 and 3. For these inequalities a table will be given which illustrates their use. The symbols of Table 7.3.4 are defined as follows:

$$U_H = S_H |U_H|, \text{ where } S_H \text{ is } +1 \text{ or } -1$$

$$A = (1 + |U_{H+H'}|)(1 + |U_{H-H'}|)$$

$$B = (1 - |U_{H+H'}|)(1 + |U_{H-H'}|)$$

$$C = (1 + |U_{H+H'}|)(1 - |U_{H-H'}|)$$

$$D = (1 - |U_{H+H'}|)(1 - |U_{H-H'}|)$$

$$\text{If } |U_{H-H'}| > |U_{H+H'}|, A > B > C > D$$

$$E = (|U_H| + |U_{H'}|)^2$$

$$F = (|U_H| - |U_{H'}|)^2$$

$$A > E > F$$

TABLE 7.3.4

Values of $S_{H+H'}$ and $S_{H-H'}$

| | |
|-------------------------|---|
| $A > E > F > B > C > D$ | Impossible |
| $A > E > B > F > C > D$ | Impossible |
| $A > E > B > C > F > D$ | Impossible |
| $A > E > B > C > D > F$ | $S_{H-H'} = S_{H+H'} - S_H S_{H'}$ |
| $A > B > E > F > C > D$ | Impossible |
| $A > B > E > C > F > D$ | $S_{H-H'} = S_H S_{H'}$ and
$S_{H+H'} = -S_H S_{H'}$ |
| $A > B > E > C > D > F$ | $S_{H-H'} = S_H S_{H'}$ |
| $A > B > C > E > F > D$ | $S_{H-H'} = -S_{H+H'}$ |
| $A > B > C > E > D > F$ | $S_{H-H'} = S_{H+H'} = S_H S_{H'}$ |
| | or $S_{H-H'} = -S_{H+H'} = S_H S_{H'}$ |
| | or $S_{H-H'} = -S_{H+H'} = -S_H S_{H'}$ |
| $A > B > C > D > E > F$ | All signs possible |

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Section 8

MISCELLANEOUS EXPONENTIAL AND TRIGONOMETRIC TABLES

| | PAGE |
|---|------|
| 8.1. THE EXPONENTIAL FUNCTION e^{-x} | 362 |
| 8.2. A FOUR-PLACE TABLE OF $\frac{\sin x}{x}$ (J. SHERMAN and L. BROCKWAY) | 366 |
| 8.3. SHORT TABLE OF $\sin 2\pi x$; $\cos 2\pi x$ | 379 |
| 8.4. TABLE OF PRODUCTS $\left\{\frac{\cos}{\sin}\right\} 2\pi x$ $\left\{\frac{\cos}{\sin}\right\} 2\pi y$ | 380 |
| 8.5. TABLE OF $\sin 2\pi hx$; $\cos 2\pi hx$ | 382 |
| 8.6. CONVERSION OF DEGREES, MINUTES AND SECONDS TO RADIANS; AND OF MINUTES AND
SECONDS TO DECIMALS OF A DEGREE; AND VICE VERSA | 430 |

8.1. The Exponential Function e^{-x}

TABLE 8.1
The Exponential Function e^{-x}

| x | ·00 | ·01 | ·02 | ·03 | ·04 | ·05 | ·06 | ·07 | ·08 | ·09 |
|-----|----------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| 0·0 | 1· 0000 | *9900 | *9802 | *9704 | *9608 | *9512 | *9418 | *9324 | *9231 | *9139 |
| 0·1 | 0· 9048 | 8958 | 8869 | 8781 | 8694 | 8607 | 8521 | 8437 | 8353 | 8270 |
| 0·2 | 0· 8187 | 8106 | 8025 | 7945 | 7866 | 7788 | 7711 | 7634 | 7558 | 7483 |
| 0·3 | 0· 7408 | 7334 | 7261 | 7189 | 7118 | 7047 | 6977 | 6907 | 6839 | 6771 |
| 0·4 | 0· 6703 | 6637 | 6570 | 6505 | 6440 | 6376 | 6313 | 6250 | 6188 | 6126 |
| 0·5 | 0· 6065 | 6005 | 5945 | 5886 | 5827 | 5769 | 5712 | 5655 | 5599 | 5543 |
| 0·6 | 0· 5488 | 5434 | 5379 | 5326 | 5273 | 5220 | 5169 | 5117 | 5066 | 5016 |
| 0·7 | 0· 4966 | 4916 | 4868 | 4819 | 4771 | 4724 | 4677 | 4630 | 4584 | 4538 |
| 0·8 | 0· 4493 | 4449 | 4404 | 4360 | 4317 | 4274 | 4232 | 4190 | 4148 | 4107 |
| 0·9 | 0· 4066 | 4025 | 3985 | 3946 | 3906 | 3867 | 3829 | 3791 | 3753 | 3716 |
| 1·0 | 0· 3679 | 3642 | 3606 | 3570 | 3535 | 3499 | 3465 | 3430 | 3396 | 3362 |
| 1·1 | 0· 3329 | 3296 | 3263 | 3230 | 3198 | 3166 | 3135 | 3104 | 3073 | 3042 |
| 1·2 | 0· 3012 | 2982 | 2952 | 2923 | 2894 | 2865 | 2837 | 2808 | 2780 | 2753 |
| 1·3 | 0· 2725 | 2698 | 2671 | 2645 | 2618 | 2592 | 2567 | 2541 | 2516 | 2491 |
| 1·4 | 0· 2466 | 2441 | 2417 | 2393 | 2369 | 2346 | 2322 | 2299 | 2276 | 2254 |
| 1·5 | 0· 2231 | 2209 | 2187 | 2165 | 2144 | 2122 | 2101 | 2080 | 2060 | 2039 |
| 1·6 | 0· 2019 | 1999 | 1979 | 1959 | 1940 | 1920 | 1901 | 1882 | 1864 | 1845 |
| 1·7 | 0· 1827 | 1809 | 1791 | 1773 | 1755 | 1738 | 1720 | 1703 | 1686 | 1670 |
| 1·8 | 0· 1653 | 1637 | 1620 | 1604 | 1588 | 1572 | 1557 | 1541 | 1526 | 1511 |
| 1·9 | 0· 1496 | 1481 | 1466 | 1451 | 1437 | 1423 | 1409 | 1395 | 1381 | 1367 |
| 2·0 | 0· 1353 | 1340 | 1327 | 1313 | 1300 | 1287 | 1275 | 1262 | 1249 | 1237 |
| 2·1 | 0· 1225 | 1212 | 1200 | 1188 | 1177 | 1165 | 1153 | 1142 | 1130 | 1119 |
| 2·2 | 0· 1108 | 1097 | 1086 | 1075 | 1065 | 1054 | 1044 | 1033 | 1023 | 1013 |
| 2·3 | 0· 1003 | *9926 | *9827 | *9730 | *9633 | *9537 | *9442 | *9348 | *9255 | *9163 |
| 2·4 | 0·0 9072 | 8981 | 8892 | 8804 | 8716 | 8629 | 8544 | 8458 | 8374 | 8291 |
| 2·5 | 0·0 8209 | 8127 | 8046 | 7966 | 7887 | 7808 | 7730 | 7654 | 7577 | 7502 |
| 2·6 | 0·0 7427 | 7353 | 7280 | 7208 | 7136 | 7065 | 6995 | 6925 | 6856 | 6788 |
| 2·7 | 0·0 6721 | 6654 | 6588 | 6522 | 6457 | 6393 | 6329 | 6266 | 6204 | 6142 |
| 2·8 | 0·0 6081 | 6020 | 5961 | 5901 | 5843 | 5784 | 5727 | 5670 | 5613 | 5558 |
| 2·9 | 0·0 5502 | 5448 | 5393 | 5340 | 5287 | 5234 | 5182 | 5130 | 5079 | 5029 |
| 3·0 | 0·0 4979 | 4929 | 4880 | 4832 | 4784 | 4736 | 4689 | 4642 | 4596 | 4550 |
| 3·1 | 0·0 4505 | 4460 | 4416 | 4372 | 4328 | 4285 | 4243 | 4200 | 4159 | 4117 |
| 3·2 | 0·0 4076 | 4036 | 3996 | 3956 | 3916 | 3877 | 3839 | 3801 | 3763 | 3725 |
| 3·3 | 0·0 3688 | 3652 | 3615 | 3579 | 3544 | 3508 | 3474 | 3439 | 3405 | 3371 |
| 3·4 | 0·0 3337 | 3304 | 3271 | 3239 | 3207 | 3175 | 3143 | 3112 | 3081 | 3050 |
| 3·5 | 0·0 3020 | 2990 | 2960 | 2930 | 2901 | 2872 | 2844 | 2816 | 2788 | 2760 |
| 3·6 | 0·0 2732 | 2705 | 2678 | 2652 | 2625 | 2599 | 2573 | 2548 | 2522 | 2497 |
| 3·7 | 0·0 2472 | 2448 | 2423 | 2399 | 2375 | 2352 | 2328 | 2305 | 2282 | 2260 |
| 3·8 | 0·0 2237 | 2215 | 2193 | 2171 | 2149 | 2128 | 2107 | 2086 | 2065 | 2045 |
| 3·9 | 0·0 2024 | 2004 | 1984 | 1964 | 1945 | 1925 | 1906 | 1887 | 1869 | 1850 |
| 4·0 | 0·0 1832 | 1813 | 1795 | 1777 | 1760 | 1742 | 1725 | 1708 | 1691 | 1674 |

8.1. THE EXPONENTIAL FUNCTION e^{-x}

TABLE 8.1 (continued)

 e^{-x}

| x | ·00 | ·01 | ·02 | ·03 | ·04 | ·05 | ·06 | ·07 | ·08 | ·09 |
|-----|------------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| 4·0 | 0·0 1832 | 1813 | 1795 | 1777 | 1760 | 1742 | 1725 | 1708 | 1691 | 1674 |
| 4·1 | 0·0 1657 | 1641 | 1624 | 1608 | 1592 | 1576 | 1561 | 1545 | 1530 | 1515 |
| 4·2 | 0·0 1500 | 1485 | 1470 | 1455 | 1441 | 1426 | 1412 | 1398 | 1384 | 1370 |
| 4·3 | 0·0 1357 | 1343 | 1330 | 1317 | 1304 | 1291 | 1278 | 1265 | 1253 | 1240 |
| 4·4 | 0·0 1228 | 1216 | 1203 | 1191 | 1180 | 1168 | 1156 | 1145 | 1133 | 1122 |
| 4·5 | 0·0 1111 | 1100 | 1089 | 1078 | 1067 | 1057 | 1046 | 1036 | 1025 | 1015 |
| 4·6 | 0·0 1005 | *9952 | *9853 | *9755 | *9658 | *9562 | *9467 | *9372 | *9279 | *9187 |
| 4·7 | 0·00 9095 | 9005 | 8915 | 8827 | 8739 | 8652 | 8566 | 8480 | 8396 | 8312 |
| 4·8 | 0·00 8230 | 8148 | 8067 | 7987 | 7907 | 7828 | 7750 | 7673 | 7597 | 7521 |
| 4·9 | 0·00 7447 | 7372 | 7299 | 7227 | 7155 | 7083 | 7013 | 6943 | 6874 | 6806 |
| 5·0 | 0·00 6738 | 6671 | 6605 | 6539 | 6474 | 6409 | 6346 | 6282 | 6220 | 6158 |
| 5·1 | 0·00 6097 | 6036 | 5976 | 5917 | 5858 | 5799 | 5742 | 5685 | 5628 | 5572 |
| 5·2 | 0·00 5517 | 5462 | 5407 | 5354 | 5300 | 5248 | 5195 | 5144 | 5092 | 5042 |
| 5·3 | 0·00 4992 | 4942 | 4893 | 4844 | 4796 | 4748 | 4701 | 4654 | 4608 | 4562 |
| 5·4 | 0·00 4517 | 4472 | 4427 | 4383 | 4339 | 4296 | 4254 | 4211 | 4169 | 4128 |
| 5·5 | 0·00 4087 | 4046 | 4006 | 3966 | 3927 | 3887 | 3849 | 3810 | 3773 | 3735 |
| 5·6 | 0·00 3698 | 3661 | 3625 | 3589 | 3553 | 3518 | 3483 | 3448 | 3414 | 3380 |
| 5·7 | 0·00 3346 | 3313 | 3280 | 3247 | 3215 | 3183 | 3151 | 3120 | 3089 | 3058 |
| 5·8 | 0·00 3028 | 2997 | 2968 | 2938 | 2909 | 2880 | 2851 | 2823 | 2795 | 2767 |
| 5·9 | 0·00 2739 | 2712 | 2685 | 2658 | 2632 | 2606 | 2580 | 2554 | 2529 | 2504 |
| 6·0 | 0·00 2479 | 2454 | 2430 | 2405 | 2382 | 2358 | 2334 | 2311 | 2288 | 2265 |
| 6·1 | 0·00 2243 | 2221 | 2198 | 2177 | 2155 | 2133 | 2112 | 2091 | 2070 | 2050 |
| 6·2 | 0·00 2029 | 2009 | 1989 | 1969 | 1950 | 1930 | 1911 | 1892 | 1873 | 1855 |
| 6·3 | 0·00 1836 | 1818 | 1800 | 1782 | 1764 | 1747 | 1729 | 1712 | 1695 | 1678 |
| 6·4 | 0·00 1662 | 1645 | 1629 | 1612 | 1596 | 1581 | 1565 | 1549 | 1534 | 1519 |
| 6·5 | 0·00 1503 | 1488 | 1474 | 1459 | 1444 | 1430 | 1416 | 1402 | 1388 | 1374 |
| 6·6 | 0·00 1360 | 1347 | 1333 | 1320 | 1307 | 1294 | 1281 | 1268 | 1256 | 1243 |
| 6·7 | 0·00 1231 | 1219 | 1207 | 1195 | 1183 | 1171 | 1159 | 1148 | 1136 | 1125 |
| 6·8 | 0·00 1114 | 1103 | 1092 | 1081 | 1070 | 1059 | 1049 | 1038 | 1028 | 1018 |
| 6·9 | 0·00 1008 | *9978 | *9878 | *9780 | *9683 | *9586 | *9491 | *9397 | *9303 | *9210 |
| 7·0 | 0·000 9119 | 9028 | 8938 | 8849 | 8761 | 8674 | 8588 | 8502 | 8418 | 8334 |
| 7·1 | 0·000 8251 | 8169 | 8088 | 8007 | 7928 | 7849 | 7771 | 7693 | 7617 | 7541 |
| 7·2 | 0·000 7466 | 7392 | 7318 | 7245 | 7173 | 7102 | 7031 | 6961 | 6892 | 6823 |
| 7·3 | 0·000 6755 | 6688 | 6622 | 6556 | 6491 | 6426 | 6362 | 6299 | 6236 | 6174 |
| 7·4 | 0·000 6113 | 6052 | 5991 | 5932 | 5873 | 5814 | 5757 | 5699 | 5643 | 5586 |
| 7·5 | 0·000 5531 | 5476 | 5421 | 5367 | 5314 | 5261 | 5209 | 5157 | 5106 | 5055 |
| 7·6 | 0·000 5005 | 4955 | 4905 | 4857 | 4808 | 4760 | 4713 | 4666 | 4620 | 4574 |
| 7·7 | 0·000 4528 | 4483 | 4439 | 4394 | 4351 | 4307 | 4265 | 4222 | 4180 | 4139 |
| 7·8 | 0·000 4097 | 4057 | 4016 | 3976 | 3937 | 3898 | 3859 | 3820 | 3782 | 3745 |
| 7·9 | 0·000 3707 | 3671 | 3634 | 3598 | 3562 | 3527 | 3492 | 3457 | 3422 | 3388 |
| 8·0 | 0·000 3355 | 3321 | 3288 | 3255 | 3223 | 3191 | 3159 | 3128 | 3097 | 3066 |

8.1. THE EXPONENTIAL FUNCTION e^{-x}

TABLE 8.1 (continued)

 e^{-x}

| x | ·00 | ·01 | ·02 | ·03 | ·04 | ·05 | ·06 | ·07 | ·08 | ·09 |
|------|--------------|------|-------|-------|-------|-------|-------|-------|-------|-------|
| 8·0 | 0·000 3355 | 3321 | 3288 | 3255 | 3223 | 3191 | 3159 | 3128 | 3097 | 3066 |
| 8·1 | 0·000 3035 | 3005 | 2975 | 2946 | 2916 | 2887 | 2859 | 2830 | 2802 | 2774 |
| 8·2 | 0·000 2747 | 2719 | 2692 | 2665 | 2639 | 2613 | 2587 | 2561 | 2535 | 2510 |
| 8·3 | 0·000 2485 | 2460 | 2436 | 2412 | 2388 | 2364 | 2340 | 2317 | 2294 | 2271 |
| 8·4 | 0·000 2249 | 2226 | 2204 | 2182 | 2161 | 2139 | 2118 | 2097 | 2076 | 2055 |
| 8·5 | 0·000 2035 | 2014 | 1994 | 1975 | 1955 | 1935 | 1916 | 1897 | 1878 | 1860 |
| 8·6 | 0·000 1841 | 1823 | 1805 | 1787 | 1769 | 1751 | 1734 | 1717 | 1700 | 1683 |
| 8·7 | 0·000 1666 | 1649 | 1633 | 1617 | 1601 | 1585 | 1569 | 1553 | 1538 | 1522 |
| 8·8 | 0·000 1507 | 1492 | 1477 | 1463 | 1448 | 1434 | 1420 | 1405 | 1391 | 1378 |
| 8·9 | 0·000 1364 | 1350 | 1337 | 1324 | 1310 | 1297 | 1284 | 1272 | 1259 | 1247 |
| 9·0 | 0·000 1234 | 1222 | 1210 | 1198 | 1186 | 1174 | 1162 | 1151 | 1139 | 1128 |
| 9·1 | 0·000 1117 | 1106 | 1095 | 1084 | 1073 | 1062 | 1052 | 1041 | 1031 | 1021 |
| 9·2 | 0·000 1010 | 1000 | *9905 | *9806 | *9709 | *9612 | *9516 | *9422 | *9328 | *9235 |
| 9·3 | 0·0000 9144 | 9052 | 8962 | 8873 | 8785 | 8697 | 8611 | 8525 | 8440 | 8356 |
| 9·4 | 0·0000 8273 | 8191 | 8109 | 8029 | 7949 | 7870 | 7792 | 7714 | 7637 | 7561 |
| 9·5 | 0·0000 7486 | 7411 | 7338 | 7265 | 7193 | 7121 | 7050 | 6980 | 6910 | 6842 |
| 9·6 | 0·0000 6774 | 6706 | 6639 | 6573 | 6508 | 6443 | 6379 | 6316 | 6253 | 6191 |
| 9·7 | 0·0000 6129 | 6068 | 6008 | 5948 | 5889 | 5830 | 5772 | 5715 | 5658 | 5601 |
| 9·8 | 0·0000 5546 | 5491 | 5436 | 5382 | 5328 | 5275 | 5223 | 5171 | 5119 | 5068 |
| 9·9 | 0·0000 5018 | 4968 | 4919 | 4870 | 4821 | 4773 | 4726 | 4679 | 4632 | 4586 |
| 10·0 | 0·0000 4540 | 4495 | 4451 | 4406 | 4362 | 4319 | 4276 | 4234 | 4191 | 4150 |
| 10·1 | 0·0000 4108 | 4068 | 4027 | 3987 | 3947 | 3908 | 3869 | 3831 | 3793 | 3755 |
| 10·2 | 0·0000 3717 | 3680 | 3644 | 3608 | 3572 | 3536 | 3501 | 3466 | 3432 | 3398 |
| 10·3 | 0·0000 3364 | 3330 | 3297 | 3264 | 3232 | 3200 | 3168 | 3136 | 3105 | 3074 |
| 10·4 | 0·0000 3044 | 3013 | 2983 | 2954 | 2924 | 2895 | 2866 | 2838 | 2810 | 2782 |
| 10·5 | 0·0000 2754 | 2727 | 2699 | 2673 | 2646 | 2620 | 2594 | 2568 | 2542 | 2517 |
| 10·6 | 0·0000 2492 | 2467 | 2443 | 2418 | 2394 | 2370 | 2347 | 2323 | 2300 | 2277 |
| 10·7 | 0·0000 2255 | 2232 | 2210 | 2188 | 2166 | 2145 | 2123 | 2102 | 2081 | 2061 |
| 10·8 | 0·0000 2040 | 2020 | 2000 | 1980 | 1960 | 1941 | 1921 | 1902 | 1883 | 1865 |
| 10·9 | 0·0000 1846 | 1828 | 1809 | 1791 | 1774 | 1756 | 1739 | 1721 | 1704 | 1687 |
| 11·0 | 0·0000 1670 | 1654 | 1637 | 1621 | 1605 | 1589 | 1573 | 1557 | 1542 | 1527 |
| 11·1 | 0·0000 1511 | 1496 | 1481 | 1467 | 1452 | 1438 | 1423 | 1409 | 1395 | 1381 |
| 11·2 | 0·0000 1368 | 1354 | 1341 | 1327 | 1314 | 1301 | 1288 | 1275 | 1262 | 1250 |
| 11·3 | 0·0000 1237 | 1225 | 1213 | 1201 | 1189 | 1177 | 1165 | 1154 | 1142 | 1131 |
| 11·4 | 0·0000 1120 | 1109 | 1098 | 1087 | 1076 | 1065 | 1054 | 1044 | 1034 | 1023 |
| 11·5 | 0·0000 1013 | 1003 | *9931 | *9832 | *9734 | *9637 | *9541 | *9446 | *9352 | *9259 |
| 11·6 | 0·00000 9167 | 9076 | 8987 | 8897 | 8808 | 8720 | 8633 | 8548 | 8462 | 8378 |
| 11·7 | 0·00000 8295 | 8212 | 8131 | 8050 | 7970 | 7890 | 7812 | 7734 | 7657 | 7581 |
| 11·8 | 0·00000 7506 | 7431 | 7357 | 7284 | 7211 | 7139 | 7068 | 6998 | 6928 | 6860 |
| 11·9 | 0·00000 6791 | 6724 | 6657 | 6591 | 6525 | 6460 | 6396 | 6332 | 6269 | 6206 |
| 12·0 | 0·00000 6144 | | | | | | | | | |

TABLE 8.1 (continued)
The Exponential Function $e^{-x}.10^p$

| x | p | .0 | .1 | .2 | .3 | .4 | .5 | .6 | .7 | .8 | .9 |
|-----|-----|------|------|-------|-------|-------|-------|-------|-------|-------|-------|
| 12 | 10 | 6144 | 5560 | 5030 | 4552 | 4119 | 3727 | 3372 | 3051 | 2761 | 2498 |
| 13 | 10 | 2260 | 2045 | 1851 | 1675 | 1515 | 1371 | 1241 | 1122 | 1016 | *9190 |
| 14 | 11 | 8315 | 7524 | 6808 | 6160 | 5574 | 5044 | 4564 | 4129 | 3737 | 3381 |
| 15 | 11 | 3059 | 2768 | 2505 | 2266 | 2051 | 1855 | 1679 | 1519 | 1375 | 1244 |
| 16 | 11 | 1125 | 1018 | *9214 | *8337 | *7544 | *6826 | *6176 | *5588 | *5057 | *4575 |

| x | p | | x | p | | x | p | | x | p | |
|-----|-----|------|-----|-----|------|-----|-----|------|-----|-----|------|
| 17 | 12 | 4140 | 21 | 14 | 7583 | 25 | 15 | 1389 | 29 | 17 | 2544 |
| 18 | 12 | 1523 | 22 | 14 | 2790 | 26 | 16 | 5109 | 30 | 18 | 9358 |
| 19 | 13 | 5603 | 23 | 14 | 1026 | 27 | 16 | 1880 | 31 | 18 | 3443 |
| 20 | 13 | 2061 | 24 | 15 | 3775 | 28 | 17 | 6914 | 32 | 18 | 1266 |

Where the Table of Proportional Parts (given on separate card) is not accurate enough for interpolation, the following method may be used:

Tabular values of function .. $f(1)$ $f(2)$ $f(3)$ $f(4)$
First differences $\Delta(12)$ $\Delta(23)$ $\Delta(34)$
Second difference $\Delta(2)$ $\Delta(3)$

Suppose it is desired to obtain a value $f(q)$ at a fraction q of the way between $f(2)$ and $f(3)$. Then

$$\begin{aligned} f(q) &= f(2) + q\Delta(23) + \frac{q(q-1)}{4}\{\Delta(2) + \Delta(3)\} \\ &= f(2) + q\Delta(23) + \frac{q(q-1)}{4}\{\Delta(34) - \Delta(12)\} \end{aligned}$$

This assumes that third differences are comparatively negligible. Alternatively, use $e^{-(a+b)} = e^{-a}.e^{-b}$ for intermediate values in the $x=a+b=12 \rightarrow 32$ range, or for higher values.

$$e^{\pm x} = 1 \pm x + \frac{x^2}{2!} \pm \frac{x^3}{3!} \pm \frac{x^4}{4!} \pm \dots$$

To find e^x , use table of e^{-x} with table of reciprocals.

To find e^x , e^{-x} for large values of x :

- 1. If $x=a+b$, $e^x=e^a \times e^b$
 $e^{-x}=e^{-a} \times e^{-b}$
- 2. $\log e^x=0.43429x$. Then use table of antilogarithms.
- 3. $\ln e^x=x$. Use table of natural logarithms inversely.

8.2. A Four-place Table of $\frac{\sin x}{x}$

By J. SHERMAN, assisted by L. BROCKWAY

Introduction

The intensities of waves diffracted by gas molecules with random orientation may be expressed by a formula of the following type:

$$I = \sum_i f_i \frac{\sin a_i x}{a_i x}$$

in which the a 's are constants and x is proportional to the sine of half the scattering angle.† The procedure which is employed for determining the structure of a single molecule by electron and X-ray diffraction experiments in the gas consists of calculating intensity curves for as many molecular models as are compatible with the known properties of the compound and then of comparing the various calculated intensity curves with the photographs, the model affording the best correlation being considered as the most probable.

In Table 8.2, $(\sin x)/x$ is given for values of the argument from 0 to 100 radians. Inasmuch as the function changes much more slowly for large values of x than for small, it was found convenient to change the value of the interval throughout the table. Accord-

ingly, for values of x from 0 to 20 radians, values of the function have been calculated for every 0.01 radian; from 20 to 40 radians, for every 0.02 radian; and from 40 to 100 radians, for every 0.05 radian.

For $x < 0.25$ radian the function was calculated by means of a Taylor's series expansion about the origin. For x between 0.25 and 6.00 radians, J. Peters' six-place table of natural sines was employed, and for x between 6.00 and 100.00 radians, O. Lohse's five-place table of natural sines was used. Table 8.2 was checked by computing first and second differences throughout. Where the second difference indicated probability of an error in the function greater than one in the last place, the value of the function was recomputed.

Inasmuch as $(\sin x)/x \leq 1$ for all values of x , values of the function multiplied by ten thousand are tabulated, to avoid the extensive use of zeros. The sign of the function is given only in the first column. Where the function changes sign, the sign is given before each value of the function throughout the row in which the change occurs.

† DEBYE, P. *Ann. Physik*, 46, 809, 1915.

TABLE 8.2A
 $\{(\sin x)/x\} \times 10^4$

| x radians | ·00 | ·01 | ·02 | ·03 | ·04 | ·05 | ·06 | ·07 | ·08 | ·09 |
|-------------|---------|-------|------|------|------|------|------|------|------|------|
| 0.0 | + 10000 | 10000 | 9999 | 9999 | 9997 | 9996 | 9994 | 9992 | 9989 | 9987 |
| 0.1 | 9983 | 9980 | 9976 | 9972 | 9967 | 9963 | 9957 | 9952 | 9946 | 9940 |
| 0.2 | 9933 | 9927 | 9919 | 9912 | 9904 | 9896 | 9889 | 9879 | 9870 | 9860 |
| 0.3 | 9851 | 9840 | 9830 | 9820 | 9808 | 9797 | 9785 | 9774 | 9761 | 9748 |
| 0.4 | 9735 | 9722 | 9709 | 9695 | 9680 | 9666 | 9651 | 9636 | 9620 | 9605 |
| 0.5 | + 9589 | 9572 | 9555 | 9538 | 9521 | 9503 | 9486 | 9467 | 9449 | 9430 |
| 0.6 | 9411 | 9391 | 9372 | 9351 | 9331 | 9311 | 9290 | 9269 | 9247 | 9225 |
| 0.7 | 9203 | 9181 | 9158 | 9135 | 9112 | 9089 | 9065 | 9041 | 9016 | 8992 |
| 0.8 | 8967 | 8942 | 8916 | 8891 | 8865 | 8839 | 8812 | 8785 | 8758 | 8731 |
| 0.9 | 8704 | 8676 | 8648 | 8620 | 8591 | 8562 | 8533 | 8504 | 8474 | 8445 |
| 1.0 | + 8415 | 8384 | 8354 | 8323 | 8292 | 8261 | 8230 | 8198 | 8166 | 8134 |
| 1.1 | 8102 | 8069 | 8037 | 8004 | 7970 | 7937 | 7903 | 7870 | 7836 | 7801 |
| 1.2 | 7767 | 7732 | 7698 | 7663 | 7627 | 7592 | 7556 | 7520 | 7484 | 7448 |
| 1.3 | 7412 | 7375 | 7339 | 7302 | 7265 | 7228 | 7190 | 7153 | 7115 | 7077 |
| 1.4 | 7039 | 7001 | 6962 | 6924 | 6885 | 6846 | 6807 | 6768 | 6729 | 6690 |
| 1.5 | + 6650 | 6610 | 6570 | 6530 | 6490 | 6450 | 6410 | 6369 | 6328 | 6288 |
| 1.6 | 6247 | 6206 | 6165 | 6124 | 6083 | 6042 | 6000 | 5959 | 5917 | 5875 |
| 1.7 | 5833 | 5791 | 5749 | 5707 | 5665 | 5623 | 5580 | 5538 | 5495 | 5453 |
| 1.8 | 5410 | 5368 | 5325 | 5282 | 5239 | 5196 | 5153 | 5110 | 5067 | 5024 |
| 1.9 | 4981 | 4937 | 4894 | 4851 | 4807 | 4764 | 4720 | 4677 | 4634 | 4590 |

8.2. A FOUR-PLACE TABLE OF $(\sin x)/x$

TABLE 8.2A (continued)

 $\{(\sin x)/x\} \times 10^4$

| x radians | ·00 | ·01 | ·02 | ·03 | ·04 | ·05 | ·06 | ·07 | ·08 | ·09 |
|-------------|-------|------|------|------|------|------|------|------|------|------|
| 2.0 | +4546 | 4503 | 4459 | 4416 | 4372 | 4329 | 4285 | 4241 | 4198 | 4153 |
| 2.1 | 4111 | 4067 | 4023 | 3980 | 3936 | 3893 | 3849 | 3805 | 3762 | 3718 |
| 2.2 | 3675 | 3632 | 3588 | 3545 | 3501 | 3458 | 3415 | 3372 | 3328 | 3285 |
| 2.3 | 3242 | 3199 | 3156 | 3113 | 3070 | 3028 | 2984 | 2942 | 2899 | 2857 |
| 2.4 | 2814 | 2772 | 2730 | 2687 | 2645 | 2603 | 2561 | 2519 | 2477 | 2436 |
| 2.5 | +2394 | 2352 | 2311 | 2269 | 2228 | 2187 | 2146 | 2105 | 2064 | 2023 |
| 2.6 | 1983 | 1942 | 1902 | 1861 | 1821 | 1781 | 1741 | 1702 | 1662 | 1622 |
| 2.7 | 1583 | 1544 | 1504 | 1465 | 1427 | 1388 | 1349 | 1311 | 1273 | 1234 |
| 2.8 | 1196 | 1159 | 1121 | 1083 | 1046 | 1009 | 972 | 935 | 898 | 861 |
| 2.9 | 825 | 789 | 753 | 717 | 681 | 646 | 610 | 575 | 540 | 505 |
| 3.0 | +470 | 436 | 402 | 368 | 334 | 300 | 266 | 233 | 200 | 167 |
| 3.1 | +134 | +102 | +69 | +37 | +5 | -27 | -58 | -90 | -121 | -152 |
| 3.2 | -182 | 213 | 243 | 273 | 303 | 333 | 362 | 392 | 421 | 449 |
| 3.3 | 478 | 506 | 535 | 562 | 590 | 618 | 645 | 672 | 699 | 725 |
| 3.4 | 752 | 778 | 804 | 829 | 855 | 880 | 905 | 930 | 954 | 978 |
| 3.5 | -1002 | 1026 | 1050 | 1073 | 1096 | 1119 | 1141 | 1164 | 1186 | 1208 |
| 3.6 | 1229 | 1251 | 1272 | 1293 | 1313 | 1334 | 1354 | 1374 | 1393 | 1413 |
| 3.7 | 1432 | 1451 | 1470 | 1488 | 1506 | 1524 | 1542 | 1559 | 1576 | 1593 |
| 3.8 | 1610 | 1627 | 1643 | 1659 | 1675 | 1690 | 1705 | 1720 | 1735 | 1749 |
| 3.9 | 1764 | 1777 | 1791 | 1805 | 1818 | 1831 | 1844 | 1856 | 1868 | 1880 |
| 4.0 | -1892 | 1903 | 1915 | 1926 | 1936 | 1947 | 1957 | 1967 | 1977 | 1987 |
| 4.1 | 1996 | 2005 | 2014 | 2022 | 2030 | 2039 | 2046 | 2054 | 2061 | 2068 |
| 4.2 | 2075 | 2082 | 2088 | 2094 | 2100 | 2106 | 2111 | 2116 | 2121 | 2126 |
| 4.3 | 2131 | 2135 | 2139 | 2143 | 2146 | 2150 | 2153 | 2156 | 2158 | 2161 |
| 4.4 | 2163 | 2165 | 2166 | 2168 | 2169 | 2170 | 2171 | 2172 | 2172 | 2172 |
| 4.5 | -2172 | 2172 | 2172 | 2171 | 2170 | 2169 | 2168 | 2166 | 2164 | 2162 |
| 4.6 | 2160 | 2158 | 2155 | 2152 | 2150 | 2146 | 2143 | 2139 | 2136 | 2132 |
| 4.7 | 2127 | 2123 | 2119 | 2114 | 2109 | 2104 | 2098 | 2093 | 2087 | 2081 |
| 4.8 | 2075 | 2069 | 2063 | 2056 | 2049 | 2042 | 2035 | 2028 | 2020 | 2013 |
| 4.9 | 2005 | 1997 | 1989 | 1981 | 1972 | 1963 | 1955 | 1946 | 1937 | 1927 |
| 5.0 | -1918 | 1908 | 1899 | 1889 | 1879 | 1868 | 1858 | 1848 | 1837 | 1826 |
| 5.1 | 1815 | 1804 | 1793 | 1782 | 1770 | 1759 | 1747 | 1735 | 1723 | 1711 |
| 5.2 | 1699 | 1687 | 1674 | 1662 | 1649 | 1636 | 1623 | 1610 | 1597 | 1584 |
| 5.3 | 1570 | 1557 | 1543 | 1530 | 1516 | 1502 | 1488 | 1474 | 1460 | 1445 |
| 5.4 | 1431 | 1417 | 1402 | 1387 | 1373 | 1358 | 1343 | 1328 | 1313 | 1298 |
| 5.5 | -1283 | 1268 | 1252 | 1237 | 1221 | 1206 | 1190 | 1175 | 1159 | 1143 |
| 5.6 | 1127 | 1111 | 1095 | 1079 | 1063 | 1047 | 1031 | 1015 | 999 | 982 |
| 5.7 | 966 | 950 | 933 | 917 | 900 | 884 | 867 | 851 | 834 | 818 |
| 5.8 | 800 | 784 | 768 | 751 | 734 | 718 | 701 | 684 | 667 | 650 |
| 5.9 | 634 | 617 | 600 | 583 | 567 | 550 | 533 | 516 | 499 | 482 |
| 6.0 | -466 | 449 | 432 | 416 | 399 | 382 | 365 | 348 | 332 | 315 |
| 6.1 | 299 | 282 | 265 | 249 | 232 | 216 | 200 | 183 | 167 | 150 |
| 6.2 | -134 | -118 | -102 | -85 | -69 | -53 | -37 | -21 | -5 | +11 |
| 6.3 | +27 | 43 | 58 | 74 | 90 | 105 | 121 | 136 | 152 | 167 |
| 6.4 | 182 | 197 | 212 | 227 | 242 | 257 | 272 | 287 | 302 | 316 |

8.2. A FOUR-PLACE TABLE OF $(\sin x)/x$

TABLE 8.2A (continued)

 $\{(\sin x)/x\} \times 10^4$

| x radians | ·00 | ·01 | ·02 | ·03 | ·04 | ·05 | ·06 | ·07 | ·08 | ·09 |
|-------------|--------|------|------|------|------|------|------|------|------|------|
| 6·5 | + 331 | 346 | 360 | 374 | 388 | 403 | 417 | 431 | 445 | 458 |
| 6·6 | 472 | 486 | 499 | 513 | 526 | 539 | 552 | 566 | 579 | 591 |
| 6·7 | 604 | 617 | 630 | 642 | 654 | 667 | 679 | 691 | 703 | 715 |
| 6·8 | 727 | 738 | 750 | 761 | 773 | 784 | 795 | 806 | 817 | 828 |
| 6·9 | 838 | 849 | 859 | 870 | 880 | 890 | 900 | 910 | 919 | 929 |
| 7·0 | + 939 | 948 | 957 | 966 | 975 | 984 | 993 | 1002 | 1010 | 1019 |
| 7·1 | 1027 | 1035 | 1043 | 1051 | 1058 | 1066 | 1074 | 1081 | 1088 | 1095 |
| 7·2 | 1102 | 1109 | 1116 | 1123 | 1129 | 1135 | 1142 | 1148 | 1153 | 1159 |
| 7·3 | 1165 | 1171 | 1176 | 1181 | 1186 | 1191 | 1196 | 1201 | 1206 | 1210 |
| 7·4 | 1214 | 1219 | 1223 | 1227 | 1231 | 1234 | 1238 | 1241 | 1244 | 1248 |
| 7·5 | + 1251 | 1254 | 1256 | 1259 | 1261 | 1264 | 1266 | 1268 | 1270 | 1272 |
| 7·6 | 1274 | 1275 | 1277 | 1278 | 1279 | 1280 | 1281 | 1282 | 1282 | 1283 |
| 7·7 | 1283 | 1284 | 1284 | 1284 | 1284 | 1283 | 1283 | 1282 | 1282 | 1281 |
| 7·8 | 1280 | 1279 | 1278 | 1277 | 1275 | 1274 | 1272 | 1270 | 1269 | 1267 |
| 7·9 | 1264 | 1262 | 1259 | 1257 | 1255 | 1252 | 1249 | 1246 | 1243 | 1240 |
| 8·0 | + 1237 | 1233 | 1230 | 1226 | 1222 | 1218 | 1214 | 1210 | 1206 | 1202 |
| 8·1 | 1197 | 1193 | 1188 | 1183 | 1179 | 1174 | 1169 | 1163 | 1158 | 1153 |
| 8·2 | 1147 | 1142 | 1136 | 1130 | 1124 | 1118 | 1112 | 1106 | 1100 | 1093 |
| 8·3 | 1087 | 1080 | 1074 | 1067 | 1060 | 1053 | 1046 | 1039 | 1032 | 1025 |
| 8·4 | 1017 | 1010 | 1002 | 995 | 987 | 979 | 972 | 964 | 956 | 948 |
| 8·5 | + 939 | 931 | 923 | 915 | 906 | 898 | 889 | 880 | 872 | 863 |
| 8·6 | 854 | 845 | 836 | 827 | 818 | 809 | 800 | 790 | 781 | 771 |
| 8·7 | 762 | 752 | 743 | 733 | 724 | 714 | 704 | 694 | 684 | 675 |
| 8·8 | 665 | 655 | 645 | 635 | 625 | 614 | 604 | 594 | 584 | 573 |
| 8·9 | 563 | 552 | 542 | 532 | 521 | 511 | 500 | 490 | 479 | 469 |
| 9·0 | + 458 | 447 | 437 | 426 | 415 | 404 | 394 | 383 | 372 | 361 |
| 9·1 | 351 | 340 | 329 | 318 | 307 | 296 | 286 | 275 | 264 | 253 |
| 9·2 | 242 | 231 | 220 | 210 | 199 | 188 | 177 | 166 | 156 | 145 |
| 9·3 | 134 | 123 | 112 | 101 | 91 | 80 | 69 | 58 | 48 | 37 |
| 9·4 | + 26 | + 16 | + 5 | − 6 | − 16 | − 27 | − 37 | − 48 | − 58 | − 69 |
| 9·5 | − 79 | 89 | 100 | 110 | 120 | 131 | 141 | 151 | 161 | 172 |
| 9·6 | 182 | 192 | 202 | 212 | 222 | 231 | 241 | 251 | 261 | 271 |
| 9·7 | 280 | 290 | 299 | 309 | 318 | 328 | 337 | 346 | 356 | 365 |
| 9·8 | 374 | 383 | 392 | 401 | 410 | 419 | 428 | 436 | 445 | 454 |
| 9·9 | 462 | 471 | 479 | 487 | 496 | 504 | 512 | 520 | 528 | 536 |
| 10·0 | − 544 | 552 | 560 | 567 | 575 | 582 | 590 | 597 | 604 | 612 |
| 10·1 | 619 | 626 | 633 | 640 | 647 | 653 | 660 | 667 | 673 | 680 |
| 10·2 | 686 | 692 | 699 | 705 | 711 | 717 | 723 | 728 | 734 | 740 |
| 10·3 | 745 | 751 | 756 | 761 | 767 | 772 | 777 | 782 | 787 | 791 |
| 10·4 | 796 | 801 | 805 | 809 | 814 | 818 | 822 | 826 | 830 | 834 |
| 10·5 | − 838 | 842 | 845 | 849 | 852 | 855 | 859 | 862 | 865 | 868 |
| 10·6 | 871 | 873 | 876 | 879 | 881 | 883 | 886 | 888 | 890 | 892 |
| 10·7 | 894 | 896 | 898 | 899 | 901 | 902 | 904 | 905 | 906 | 907 |
| 10·8 | 908 | 909 | 910 | 911 | 911 | 912 | 912 | 913 | 913 | 913 |
| 10·9 | 913 | 913 | 913 | 913 | 913 | 912 | 912 | 911 | 911 | 910 |

8.2. A FOUR-PLACE TABLE OF $(\sin x)/x$

TABLE 8.2A (continued)
 $\{(\sin x)/x\} \times 10^4$

| x radians | ·00 | ·01 | ·02 | ·03 | ·04 | ·05 | ·06 | ·07 | ·08 | ·09 |
|-----------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| 11·0 | −909 | 908 | 907 | 906 | 905 | 904 | 902 | 901 | 899 | 898 |
| 11·1 | 896 | 894 | 892 | 890 | 888 | 886 | 884 | 882 | 879 | 877 |
| 11·2 | 874 | 872 | 869 | 866 | 863 | 860 | 857 | 854 | 851 | 848 |
| 11·3 | 844 | 841 | 837 | 834 | 830 | 826 | 822 | 819 | 815 | 811 |
| 11·4 | 806 | 802 | 798 | 794 | 789 | 785 | 780 | 776 | 771 | 766 |
| 11·5 | −761 | 756 | 751 | 746 | 741 | 736 | 731 | 726 | 720 | 715 |
| 11·6 | 709 | 704 | 698 | 693 | 687 | 681 | 675 | 669 | 663 | 657 |
| 11·7 | 651 | 645 | 639 | 633 | 626 | 620 | 614 | 607 | 601 | 594 |
| 11·8 | 588 | 581 | 574 | 568 | 561 | 554 | 547 | 540 | 533 | 526 |
| 11·9 | 519 | 512 | 505 | 498 | 491 | 484 | 476 | 469 | 462 | 454 |
| 12·0 | −447 | 440 | 432 | 425 | 417 | 410 | 402 | 395 | 387 | 379 |
| 12·1 | 372 | 364 | 356 | 348 | 341 | 333 | 325 | 317 | 309 | 301 |
| 12·2 | 294 | 286 | 278 | 270 | 262 | 254 | 246 | 238 | 230 | 222 |
| 12·3 | 214 | 206 | 198 | 190 | 182 | 174 | 166 | 158 | 150 | 142 |
| 12·4 | 134 | 125 | 117 | 109 | 101 | 93 | 85 | 77 | 69 | 61 |
| 12·5 | −53 | −45 | −37 | −29 | −21 | −13 | −5 | +3 | +11 | +19 |
| 12·6 | +27 | 35 | 42 | 50 | 58 | 66 | 74 | 82 | 89 | 97 |
| 12·7 | 105 | 113 | 120 | 128 | 136 | 143 | 151 | 158 | 166 | 173 |
| 12·8 | 181 | 188 | 196 | 203 | 210 | 218 | 225 | 232 | 240 | 247 |
| 12·9 | 254 | 261 | 268 | 275 | 282 | 289 | 296 | 303 | 310 | 316 |
| 13·0 | +323 | 330 | 337 | 343 | 350 | 356 | 363 | 369 | 376 | 382 |
| 13·1 | 388 | 395 | 401 | 407 | 413 | 419 | 425 | 431 | 437 | 443 |
| 13·2 | 448 | 454 | 460 | 466 | 471 | 477 | 482 | 488 | 493 | 498 |
| 13·3 | 503 | 509 | 514 | 519 | 524 | 529 | 534 | 538 | 543 | 548 |
| 13·4 | 552 | 557 | 562 | 566 | 570 | 575 | 579 | 583 | 587 | 591 |
| 13·5 | +595 | 599 | 603 | 607 | 611 | 614 | 618 | 622 | 625 | 628 |
| 13·6 | 632 | 635 | 638 | 641 | 644 | 647 | 650 | 653 | 656 | 659 |
| 13·7 | 661 | 664 | 666 | 669 | 671 | 673 | 676 | 678 | 680 | 682 |
| 13·8 | 684 | 686 | 688 | 689 | 691 | 692 | 694 | 695 | 697 | 698 |
| 13·9 | 699 | 700 | 702 | 703 | 703 | 704 | 705 | 706 | 706 | 707 |
| 14·0 | +708 | 708 | 708 | 709 | 709 | 709 | 709 | 709 | 709 | 709 |
| 14·1 | 709 | 708 | 708 | 708 | 707 | 707 | 706 | 705 | 705 | 704 |
| 14·2 | 703 | 702 | 701 | 700 | 699 | 697 | 696 | 695 | 693 | 692 |
| 14·3 | 690 | 688 | 687 | 685 | 683 | 681 | 679 | 677 | 675 | 673 |
| 14·4 | 671 | 668 | 666 | 663 | 661 | 658 | 656 | 653 | 650 | 648 |
| 14·5 | +645 | 642 | 639 | 636 | 633 | 630 | 626 | 623 | 620 | 616 |
| 14·6 | 613 | 609 | 606 | 602 | 599 | 595 | 591 | 587 | 583 | 579 |
| 14·7 | 575 | 571 | 567 | 563 | 559 | 555 | 550 | 546 | 542 | 537 |
| 14·8 | 533 | 528 | 524 | 519 | 514 | 509 | 505 | 500 | 495 | 490 |
| 14·9 | 485 | 480 | 475 | 470 | 465 | 460 | 455 | 449 | 444 | 439 |
| 15·0 | +434 | 428 | 423 | 417 | 412 | 406 | 401 | 395 | 390 | 384 |
| 15·1 | 378 | 373 | 367 | 361 | 355 | 349 | 344 | 338 | 332 | 326 |
| 15·2 | 320 | 314 | 308 | 302 | 296 | 290 | 284 | 278 | 272 | 265 |
| 15·3 | 259 | 253 | 247 | 241 | 234 | 228 | 222 | 216 | 209 | 203 |
| 15·4 | 197 | 190 | 184 | 178 | 171 | 165 | 159 | 152 | 146 | 140 |

8.2. A FOUR-PLACE TABLE OF $(\sin x)/x$

TABLE 8.2A (continued)

 $\{(\sin x)/x\} \times 10^4$

| x radians | ·00 | ·01 | ·02 | ·03 | ·04 | ·05 | ·06 | ·07 | ·08 | ·09 |
|-------------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| 15.5 | +133 | 127 | 120 | 114 | 108 | 101 | 95 | 88 | 82 | 76 |
| 15.6 | 69 | 63 | 56 | 50 | 43 | 37 | 31 | 24 | 18 | 11 |
| 15.7 | +5 | -1 | -8 | -14 | -20 | -27 | -33 | -39 | -46 | -52 |
| 15.8 | 58 | 64 | 71 | 77 | 83 | 89 | 95 | 102 | 108 | 114 |
| 15.9 | 120 | 126 | 132 | 138 | 144 | 150 | 156 | 162 | 168 | 174 |
| 16.0 | -180 | 186 | 192 | 197 | 203 | 209 | 215 | 220 | 226 | 232 |
| 16.1 | 237 | 243 | 248 | 254 | 259 | 265 | 270 | 276 | 281 | 286 |
| 16.2 | 292 | 297 | 302 | 307 | 312 | 318 | 323 | 328 | 333 | 337 |
| 16.3 | 342 | 347 | 352 | 357 | 362 | 366 | 371 | 376 | 380 | 385 |
| 16.4 | 389 | 393 | 398 | 402 | 407 | 411 | 415 | 419 | 423 | 427 |
| 16.5 | -431 | 435 | 439 | 443 | 447 | 451 | 454 | 458 | 462 | 465 |
| 16.6 | 469 | 472 | 476 | 479 | 482 | 486 | 489 | 492 | 495 | 498 |
| 16.7 | 501 | 504 | 507 | 510 | 513 | 515 | 518 | 521 | 523 | 526 |
| 16.8 | 528 | 531 | 533 | 535 | 538 | 540 | 542 | 544 | 546 | 548 |
| 16.9 | 550 | 552 | 553 | 555 | 557 | 558 | 560 | 561 | 563 | 564 |
| 17.0 | -566 | 567 | 568 | 569 | 570 | 571 | 572 | 573 | 574 | 575 |
| 17.1 | 575 | 576 | 577 | 577 | 578 | 578 | 579 | 579 | 579 | 579 |
| 17.2 | 580 | 580 | 580 | 580 | 580 | 579 | 579 | 579 | 579 | 578 |
| 17.3 | 578 | 577 | 577 | 576 | 576 | 575 | 574 | 573 | 572 | 571 |
| 17.4 | 570 | 569 | 568 | 567 | 566 | 565 | 563 | 562 | 561 | 559 |
| 17.5 | -557 | 556 | 554 | 553 | 551 | 549 | 547 | 545 | 543 | 541 |
| 17.6 | 539 | 537 | 535 | 533 | 530 | 528 | 526 | 523 | 521 | 518 |
| 17.7 | 516 | 513 | 510 | 508 | 505 | 502 | 499 | 496 | 493 | 490 |
| 17.8 | 487 | 484 | 481 | 478 | 475 | 471 | 468 | 465 | 461 | 458 |
| 17.9 | 454 | 451 | 447 | 444 | 440 | 436 | 433 | 429 | 425 | 421 |
| 18.0 | -417 | 413 | 409 | 405 | 401 | 397 | 393 | 389 | 385 | 381 |
| 18.1 | 376 | 372 | 368 | 364 | 359 | 355 | 350 | 346 | 341 | 337 |
| 18.2 | 332 | 328 | 323 | 319 | 314 | 309 | 304 | 300 | 295 | 290 |
| 18.3 | 285 | 281 | 276 | 271 | 266 | 261 | 256 | 251 | 246 | 241 |
| 18.4 | 236 | 231 | 226 | 221 | 216 | 211 | 206 | 201 | 195 | 190 |
| 18.5 | -185 | 180 | 175 | 170 | 164 | 159 | 154 | 149 | 143 | 138 |
| 18.6 | 133 | 128 | 122 | 117 | 112 | 106 | 101 | 96 | 90 | 85 |
| 18.7 | 80 | 74 | 69 | 64 | 58 | 53 | 48 | 42 | 37 | 32 |
| 18.8 | -26 | -21 | -16 | -10 | -5 | +0 | +6 | +11 | +16 | +21 |
| 18.9 | +27 | 32 | 37 | 42 | 48 | 53 | 58 | 63 | 68 | 74 |
| 19.0 | +79 | 84 | 89 | 94 | 99 | 104 | 110 | 115 | 120 | 125 |
| 19.1 | 130 | 135 | 140 | 145 | 150 | 155 | 159 | 164 | 169 | 174 |
| 19.2 | 179 | 184 | 188 | 193 | 198 | 202 | 207 | 212 | 216 | 221 |
| 19.3 | 226 | 230 | 235 | 239 | 244 | 248 | 252 | 257 | 261 | 265 |
| 19.4 | 270 | 274 | 278 | 282 | 286 | 290 | 295 | 299 | 303 | 307 |
| 19.5 | +311 | 314 | 318 | 322 | 326 | 330 | 333 | 337 | 341 | 344 |
| 19.6 | 348 | 351 | 355 | 358 | 362 | 365 | 369 | 372 | 375 | 378 |
| 19.7 | 382 | 385 | 388 | 391 | 394 | 397 | 400 | 403 | 405 | 408 |
| 19.8 | 411 | 414 | 416 | 419 | 422 | 424 | 427 | 429 | 431 | 434 |
| 19.9 | 436 | 438 | 440 | 443 | 445 | 447 | 449 | 451 | 453 | 455 |

8.2. A FOUR-PLACE TABLE OF $(\sin x)/x$ TABLE 8.2B
 $\{(\sin x)/x\} \times 10^4$

| x radians | ·00 | ·02 | ·04 | ·06 | ·08 | x radians | ·00 | ·02 | ·04 | ·06 | ·08 |
|-------------|------|-----|-----|-----|-----|-------------|------|-----|-----|-----|-----|
| 20·0 | +456 | 460 | 463 | 466 | 469 | 24·5 | −241 | 235 | 228 | 221 | 214 |
| 20·1 | 472 | 475 | 477 | 479 | 481 | 24·6 | 206 | 199 | 192 | 185 | 177 |
| 20·2 | 483 | 485 | 486 | 487 | 488 | 24·7 | 170 | 162 | 155 | 147 | 139 |
| 20·3 | 489 | 490 | 490 | 490 | 490 | 24·8 | 132 | 124 | 116 | 108 | 100 |
| 20·4 | 490 | 490 | 489 | 488 | 487 | 24·9 | 93 | 85 | 77 | 69 | 61 |
| 20·5 | +486 | 485 | 483 | 482 | 480 | 25·0 | −53 | 45 | 37 | 29 | 21 |
| 20·6 | 478 | 475 | 473 | 470 | 467 | 25·1 | −13 | −5 | +3 | +11 | +19 |
| 20·7 | 464 | 461 | 458 | 454 | 450 | 25·2 | +27 | 35 | 42 | 50 | 58 |
| 20·8 | 447 | 442 | 438 | 434 | 429 | 25·3 | 66 | 74 | 81 | 89 | 96 |
| 20·9 | 424 | 420 | 415 | 409 | 404 | 25·4 | 104 | 111 | 119 | 126 | 134 |
| 21·0 | +398 | 393 | 387 | 381 | 375 | 25·5 | +141 | 148 | 155 | 162 | 169 |
| 21·1 | 369 | 362 | 356 | 349 | 342 | 25·6 | 176 | 183 | 189 | 196 | 203 |
| 21·2 | 335 | 328 | 321 | 314 | 307 | 25·7 | 209 | 215 | 222 | 228 | 234 |
| 21·3 | 299 | 292 | 284 | 276 | 268 | 25·8 | 240 | 246 | 251 | 257 | 263 |
| 21·4 | 260 | 252 | 244 | 236 | 228 | 25·9 | 268 | 273 | 278 | 284 | 288 |
| 21·5 | +219 | 211 | 202 | 194 | 185 | 26·0 | +293 | 298 | 303 | 307 | 311 |
| 21·6 | 176 | 168 | 159 | 150 | 141 | 26·1 | 315 | 320 | 323 | 327 | 331 |
| 21·7 | 132 | 123 | 114 | 105 | 96 | 26·2 | 334 | 338 | 341 | 344 | 347 |
| 21·8 | 87 | 78 | 69 | 60 | 51 | 26·3 | 350 | 352 | 355 | 357 | 359 |
| 21·9 | 42 | 32 | 23 | 14 | 5 | 26·4 | 361 | 363 | 365 | 367 | 368 |
| 22·0 | −4 | 13 | 22 | 31 | 40 | 26·5 | +370 | 371 | 372 | 373 | 373 |
| 22·1 | 49 | 58 | 67 | 76 | 85 | 26·6 | 374 | 374 | 375 | 375 | 375 |
| 22·2 | 93 | 102 | 111 | 119 | 128 | 26·7 | 375 | 374 | 374 | 373 | 372 |
| 22·3 | 136 | 145 | 153 | 161 | 169 | 26·8 | 371 | 370 | 369 | 368 | 366 |
| 22·4 | 178 | 185 | 193 | 201 | 209 | 26·9 | 365 | 363 | 361 | 359 | 357 |
| 22·5 | −217 | 224 | 231 | 239 | 246 | 27·0 | +354 | 352 | 349 | 346 | 343 |
| 22·6 | 253 | 260 | 267 | 274 | 280 | 27·1 | 340 | 337 | 334 | 331 | 327 |
| 22·7 | 287 | 293 | 299 | 305 | 311 | 27·2 | 323 | 319 | 316 | 312 | 307 |
| 22·8 | 317 | 323 | 329 | 334 | 339 | 27·3 | 303 | 299 | 294 | 290 | 285 |
| 22·9 | 344 | 349 | 354 | 359 | 364 | 27·4 | 280 | 275 | 270 | 265 | 260 |
| 23·0 | −368 | 372 | 376 | 380 | 384 | 27·5 | +254 | 249 | 243 | 238 | 232 |
| 23·1 | 388 | 391 | 394 | 397 | 400 | 27·6 | 226 | 220 | 214 | 208 | 202 |
| 23·2 | 403 | 406 | 408 | 410 | 413 | 27·7 | 196 | 190 | 184 | 177 | 171 |
| 23·3 | 415 | 416 | 418 | 419 | 421 | 27·8 | 164 | 158 | 151 | 145 | 138 |
| 23·4 | 422 | 423 | 423 | 424 | 424 | 27·9 | 131 | 124 | 117 | 111 | 104 |
| 23·5 | −425 | 425 | 425 | 424 | 424 | 28·0 | +97 | 90 | 83 | 76 | 69 |
| 23·6 | 423 | 423 | 422 | 421 | 419 | 28·1 | 62 | 55 | 48 | 41 | 34 |
| 23·7 | 418 | 416 | 415 | 413 | 411 | 28·2 | +26 | +19 | +12 | +5 | −2 |
| 23·8 | 408 | 406 | 403 | 401 | 398 | 28·3 | −9 | 16 | 23 | 30 | 37 |
| 23·9 | 395 | 392 | 388 | 385 | 381 | 28·4 | 44 | 51 | 58 | 65 | 72 |
| 24·0 | −377 | 373 | 369 | 365 | 361 | 28·5 | −79 | 85 | 92 | 99 | 105 |
| 24·1 | 356 | 352 | 347 | 342 | 337 | 28·6 | 112 | 118 | 125 | 131 | 138 |
| 24·2 | 332 | 327 | 321 | 316 | 310 | 28·7 | 144 | 150 | 156 | 162 | 168 |
| 24·3 | 304 | 299 | 293 | 287 | 280 | 28·8 | 174 | 180 | 186 | 192 | 197 |
| 24·4 | 274 | 268 | 261 | 255 | 248 | 28·9 | 203 | 208 | 213 | 219 | 224 |

8.2. A FOUR-PLACE TABLE OF $(\sin x)/x$

TABLE 8.2B (continued)

 $\{(\sin x)/x\} \times 10^4$

| x radians | ·00 | ·02 | ·04 | ·06 | ·08 | x radians | ·00 | ·02 | ·04 | ·06 | ·08 |
|-------------|------|-----|-----|-----|-----|-------------|------|-----|-----|-----|-----|
| 29.0 | -229 | 234 | 239 | 243 | 248 | 33.5 | +260 | 257 | 254 | 250 | 247 |
| 29.1 | 253 | 257 | 261 | 266 | 270 | 33.6 | 243 | 240 | 236 | 232 | 228 |
| 29.2 | 274 | 278 | 281 | 285 | 288 | 33.7 | 224 | 220 | 216 | 212 | 208 |
| 29.3 | 292 | 295 | 298 | 301 | 304 | 33.8 | 203 | 199 | 194 | 190 | 185 |
| 29.4 | 307 | 310 | 312 | 315 | 317 | 33.9 | 180 | 175 | 171 | 166 | 161 |
| 29.5 | -319 | 321 | 323 | 325 | 326 | 34.0 | +156 | 151 | 145 | 140 | 135 |
| 29.6 | 328 | 329 | 330 | 331 | 332 | 34.1 | 130 | 124 | 119 | 113 | 108 |
| 29.7 | 333 | 334 | 334 | 335 | 335 | 34.2 | 102 | 97 | 91 | 86 | 80 |
| 29.8 | 335 | 335 | 335 | 335 | 334 | 34.3 | 74 | 69 | 63 | 57 | 51 |
| 29.9 | 334 | 333 | 332 | 332 | 331 | 34.4 | 46 | 40 | 34 | 28 | 22 |
| 30.0 | -329 | 328 | 327 | 325 | 323 | 34.5 | +17 | +11 | +5 | -1 | -7 |
| 30.1 | 321 | 320 | 317 | 315 | 313 | 34.6 | -12 | 18 | 24 | 30 | 35 |
| 30.2 | 311 | 308 | 305 | 302 | 300 | 34.7 | 41 | 47 | 52 | 58 | 63 |
| 30.3 | 296 | 293 | 290 | 287 | 283 | 34.8 | 69 | 75 | 80 | 85 | 91 |
| 30.4 | 280 | 276 | 272 | 268 | 264 | 34.9 | 96 | 102 | 107 | 112 | 117 |
| 30.5 | -260 | 256 | 252 | 247 | 243 | 35.0 | -122 | 127 | 132 | 137 | 142 |
| 30.6 | 238 | 233 | 229 | 224 | 219 | 35.1 | 147 | 152 | 157 | 161 | 166 |
| 30.7 | 214 | 209 | 204 | 198 | 193 | 35.2 | 170 | 175 | 179 | 183 | 187 |
| 30.8 | 188 | 182 | 177 | 171 | 165 | 35.3 | 192 | 196 | 199 | 203 | 207 |
| 30.9 | 160 | 154 | 148 | 142 | 136 | 35.4 | 211 | 214 | 218 | 221 | 225 |
| 31.0 | -130 | 124 | 118 | 112 | 106 | 35.5 | -228 | 231 | 234 | 237 | 240 |
| 31.1 | 100 | 94 | 87 | 81 | 75 | 35.6 | 243 | 245 | 248 | 250 | 253 |
| 31.2 | 69 | 62 | 56 | 50 | 43 | 35.7 | 255 | 257 | 259 | 261 | 263 |
| 31.3 | 37 | 31 | 24 | 18 | 11 | 35.8 | 264 | 266 | 268 | 269 | 270 |
| 31.4 | -5 | +1 | +8 | +14 | +20 | 35.9 | 271 | 272 | 273 | 274 | 275 |
| 31.5 | +27 | 33 | 39 | 45 | 52 | 36.0 | -275 | 276 | 276 | 277 | 277 |
| 31.6 | 58 | 64 | 70 | 76 | 82 | 36.1 | 277 | 277 | 277 | 276 | 276 |
| 31.7 | 88 | 94 | 100 | 106 | 112 | 36.2 | 276 | 275 | 274 | 273 | 272 |
| 31.8 | 118 | 124 | 129 | 135 | 140 | 36.3 | 271 | 270 | 269 | 268 | 266 |
| 31.9 | 146 | 151 | 157 | 162 | 167 | 36.4 | 265 | 263 | 261 | 259 | 257 |
| 32.0 | +172 | 177 | 182 | 187 | 192 | 36.5 | -255 | 253 | 251 | 248 | 246 |
| 32.1 | 197 | 202 | 206 | 211 | 215 | 36.6 | 243 | 241 | 238 | 235 | 232 |
| 32.2 | 219 | 224 | 228 | 232 | 236 | 36.7 | 229 | 226 | 223 | 220 | 216 |
| 32.3 | 239 | 243 | 247 | 250 | 254 | 36.8 | 213 | 209 | 206 | 202 | 198 |
| 32.4 | 257 | 260 | 263 | 266 | 269 | 36.9 | 194 | 190 | 186 | 182 | 178 |
| 32.5 | +272 | 275 | 277 | 280 | 282 | 37.0 | -174 | 170 | 165 | 161 | 156 |
| 32.6 | 284 | 286 | 288 | 290 | 292 | 37.1 | 152 | 147 | 143 | 138 | 133 |
| 32.7 | 293 | 295 | 296 | 297 | 299 | 37.2 | 129 | 124 | 119 | 114 | 109 |
| 32.8 | 300 | 300 | 301 | 302 | 302 | 37.3 | 104 | 99 | 94 | 89 | 84 |
| 32.9 | 303 | 303 | 303 | 303 | 303 | 37.4 | 79 | 74 | 68 | 63 | 58 |
| 33.0 | +303 | 303 | 302 | 302 | 301 | 37.5 | -53 | 47 | 42 | 37 | 32 |
| 33.1 | 300 | 299 | 298 | 297 | 296 | 37.6 | 26 | 21 | 16 | 10 | 5 |
| 33.2 | 294 | 293 | 291 | 290 | 288 | 37.7 | +0 | 6 | 11 | 16 | 21 |
| 33.3 | 286 | 284 | 281 | 279 | 277 | 37.8 | 27 | 32 | 37 | 42 | 47 |
| 33.4 | 274 | 272 | 269 | 266 | 263 | 37.9 | 53 | 58 | 63 | 68 | 73 |

8.2. A FOUR-PLACE TABLE OF $(\sin x)/x$

TABLE 8.2B (continued)

$\{(\sin x)/x\} \times 10^4$

| x radians | ·00 | ·02 | ·04 | ·06 | ·08 | x radians | ·00 | ·02 | ·04 | ·06 | ·08 |
|-------------|-------|-----|-----|-----|-----|-------------|-------|-----|-----|-----|-----|
| 38·0 | + 78 | 83 | 88 | 93 | 98 | 39·0 | + 247 | 248 | 249 | 250 | 251 |
| 38·1 | 102 | 107 | 112 | 117 | 121 | 39·1 | 252 | 253 | 253 | 254 | 254 |
| 38·2 | 126 | 130 | 135 | 139 | 143 | 39·2 | 254 | 255 | 255 | 255 | 255 |
| 38·3 | 148 | 152 | 156 | 160 | 164 | 39·3 | 254 | 254 | 254 | 253 | 252 |
| 38·4 | 168 | 172 | 176 | 179 | 183 | 39·4 | 252 | 251 | 250 | 249 | 248 |
| 38·5 | + 186 | 190 | 193 | 197 | 200 | 39·5 | + 246 | 245 | 244 | 242 | 241 |
| 38·6 | 203 | 206 | 209 | 212 | 215 | 39·6 | 239 | 237 | 235 | 233 | 231 |
| 38·7 | 218 | 220 | 223 | 225 | 228 | 39·7 | 229 | 227 | 224 | 222 | 219 |
| 38·8 | 230 | 232 | 234 | 236 | 238 | 39·8 | 217 | 214 | 211 | 208 | 206 |
| 38·9 | 240 | 241 | 243 | 244 | 246 | 39·9 | 203 | 199 | 196 | 193 | 190 |

TABLE 8.2C

$\{(\sin x)/x\} \times 10^4$

| x
radians | $\frac{\sin x}{x}$ | x
radians | $\frac{\sin x}{x}$ | x
radians | $\frac{\sin x}{x}$ | x
radians | $\frac{\sin x}{x}$ | x
radians | $\frac{\sin x}{x}$ |
|----------------|--------------------|----------------|--------------------|----------------|--------------------|----------------|--------------------|----------------|--------------------|
| 40·00 | + 186 | 41·25 | −96 | 42·50 | −234 | 43·75 | −53 | 45·00 | + 189 |
| ·05 | 177 | ·30 | 107 | ·55 | 233 | ·80 | 41 | ·05 | 194 |
| ·10 | 168 | ·35 | 118 | ·60 | 231 | ·85 | 30 | ·10 | 199 |
| ·15 | 159 | ·40 | 128 | ·65 | 228 | ·90 | 19 | ·15 | 204 |
| ·20 | 149 | ·45 | 138 | ·70 | 225 | ·95 | 7 | ·20 | 208 |
| 40·25 | + 138 | 41·50 | −148 | 42·75 | −221 | 44·00 | + 4 | 45·25 | + 211 |
| ·30 | 128 | ·55 | 157 | ·80 | 216 | ·05 | 15 | ·30 | 214 |
| ·35 | 117 | ·60 | 165 | ·85 | 211 | ·10 | 27 | ·35 | 216 |
| ·40 | 106 | ·65 | 174 | ·90 | 206 | ·15 | 38 | ·40 | 218 |
| ·45 | 94 | ·70 | 182 | ·95 | 200 | ·20 | 49 | ·45 | 219 |
| 40·50 | + 83 | 41·75 | −189 | 43·00 | −193 | 44·25 | + 60 | 45·50 | + 219 |
| ·55 | 71 | ·80 | 196 | ·05 | 187 | ·30 | 71 | ·55 | 220 |
| ·60 | 59 | ·85 | 202 | ·10 | 179 | ·35 | 81 | ·60 | 219 |
| ·65 | 47 | ·90 | 208 | ·15 | 171 | ·40 | 91 | ·65 | 218 |
| ·70 | 34 | ·95 | 213 | ·20 | 163 | ·45 | 101 | ·70 | 216 |
| 40·75 | + 22 | 42·00 | −218 | 43·25 | −155 | 44·50 | + 111 | 45·75 | + 214 |
| ·80 | + 10 | ·05 | 222 | ·30 | 146 | ·55 | 121 | ·80 | 212 |
| ·85 | −2 | ·10 | 226 | ·35 | 136 | ·60 | 130 | ·85 | 209 |
| ·90 | 15 | ·15 | 229 | ·40 | 127 | ·65 | 139 | ·90 | 205 |
| ·95 | 27 | ·20 | 232 | ·45 | 117 | ·70 | 147 | ·95 | 201 |
| 41·00 | −39 | 42·25 | −234 | 43·50 | −107 | 44·75 | + 155 | 46·00 | + 196 |
| ·05 | 51 | ·30 | 235 | ·55 | 96 | ·80 | 163 | ·05 | 191 |
| ·10 | 62 | ·35 | 236 | ·60 | 86 | ·85 | 170 | ·10 | 185 |
| ·15 | 74 | ·40 | 236 | ·65 | 75 | ·90 | 177 | ·15 | 179 |
| ·20 | 85 | ·45 | 235 | ·70 | 64 | ·95 | 183 | ·20 | 173 |

8.2. A FOUR-PLACE TABLE OF $(\sin x)/x$

TABLE 8.2C (continued)

 $\{(\sin x)/x\} \times 10^4$

| x
radians | $\frac{\sin x}{x}$ | x
radians | $\frac{\sin x}{x}$ | x
radians | $\frac{\sin x}{x}$ | x
radians | $\frac{\sin x}{x}$ | x
radians | $\frac{\sin x}{x}$ |
|----------------|--------------------|----------------|--------------------|----------------|--------------------|----------------|--------------------|----------------|--------------------|
| 46.25 | +166 | 48.50 | -202 | 50.75 | +92 | 53.00 | +75 | 55.25 | -174 |
| .30 | 158 | .55 | 204 | .80 | 100 | .05 | 66 | .30 | 172 |
| .35 | 151 | .60 | 205 | .85 | 109 | .10 | 57 | .35 | 168 |
| .40 | 143 | .65 | 205 | .90 | 116 | .15 | 48 | .40 | 165 |
| .45 | 134 | .70 | 205 | .95 | 124 | .20 | 39 | .45 | 161 |
| 46.50 | +126 | 48.75 | -205 | 51.00 | +131 | 53.25 | +29 | 55.50 | -156 |
| .55 | 117 | .80 | 204 | .05 | 138 | .30 | 20 | .55 | 151 |
| .60 | 107 | .85 | 202 | .10 | 145 | .35 | 11 | .60 | 146 |
| .65 | 98 | .90 | 200 | .15 | 151 | .40 | +1 | .65 | 141 |
| .70 | 88 | .95 | 198 | .20 | 157 | .45 | -8 | .70 | 135 |
| 46.75 | +78 | 49.00 | -195 | 51.25 | +163 | 53.50 | -17 | 55.75 | -129 |
| .80 | 68 | .05 | 191 | .30 | 168 | .55 | 27 | .80 | 122 |
| .85 | 58 | .10 | 187 | .35 | 172 | .60 | 36 | .85 | 115 |
| .90 | 47 | .15 | 183 | .40 | 176 | .65 | 45 | .90 | 108 |
| .95 | 37 | .20 | 178 | .45 | 180 | .70 | 54 | .95 | 101 |
| 47.00 | +26 | 49.25 | -173 | 51.50 | +183 | 53.75 | -63 | 56.00 | -93 |
| .05 | 16 | .30 | 167 | .55 | 186 | .80 | 71 | .05 | 85 |
| .10 | +5 | .35 | 161 | .60 | 188 | .85 | 80 | .10 | 77 |
| .15 | -6 | .40 | 154 | .65 | 190 | .90 | 88 | .15 | 69 |
| .20 | 16 | .45 | 147 | .70 | 192 | .95 | 96 | .20 | 61 |
| 47.25 | -27 | 49.50 | -140 | 51.75 | +193 | 54.00 | -103 | 56.25 | -52 |
| .30 | 37 | .55 | 132 | .80 | 193 | .05 | 111 | .30 | 44 |
| .35 | 47 | .60 | 124 | .85 | 193 | .10 | 118 | .35 | 35 |
| .40 | 58 | .65 | 116 | .90 | 192 | .15 | 125 | .40 | 26 |
| .45 | 67 | .70 | 108 | .95 | 191 | .20 | 131 | .45 | 17 |
| 47.50 | -77 | 49.75 | -99 | 52.00 | +190 | 54.25 | -138 | 56.50 | -9 |
| .55 | 87 | .80 | 90 | .05 | 188 | .30 | 143 | .55 | +0 |
| .60 | 96 | .85 | 81 | .10 | 185 | .35 | 149 | .60 | 9 |
| .65 | 105 | .90 | 72 | .15 | 182 | .40 | 154 | .65 | 18 |
| .70 | 114 | .95 | 62 | .20 | 179 | .45 | 159 | .70 | 27 |
| 47.75 | -123 | 50.00 | -52 | 52.25 | +175 | 54.50 | -163 | 56.75 | +35 |
| .80 | 131 | .05 | 43 | .30 | 171 | .55 | 167 | .80 | 44 |
| .85 | 139 | .10 | 33 | .35 | 166 | .60 | 170 | .85 | 52 |
| .90 | 146 | .15 | 23 | .40 | 161 | .65 | 173 | .90 | 60 |
| .95 | 153 | .20 | 13 | .45 | 156 | .70 | 176 | .95 | 69 |
| 48.00 | -160 | 50.25 | -3 | 52.50 | +150 | 54.75 | -178 | 57.00 | +77 |
| .05 | 166 | .30 | +7 | .55 | 144 | .80 | 180 | .05 | 84 |
| .10 | 172 | .35 | 17 | .60 | 137 | .85 | 181 | .10 | 92 |
| .15 | 178 | .40 | 27 | .65 | 130 | .90 | 182 | .15 | 99 |
| .20 | 183 | .45 | 36 | .70 | 123 | .95 | 182 | .20 | 106 |
| 48.25 | -187 | 50.50 | +46 | 52.75 | +116 | 55.00 | -182 | 57.25 | +113 |
| .30 | 191 | .55 | 56 | .80 | 108 | .05 | 181 | .30 | 119 |
| .35 | 195 | .60 | 65 | .85 | 100 | .10 | 180 | .35 | 125 |
| .40 | 198 | .65 | 74 | .90 | 92 | .15 | 179 | .40 | 131 |
| .45 | 200 | .70 | 83 | .95 | 83 | .20 | 177 | .45 | 136 |

8.2. A FOUR-PLACE TABLE OF $(\sin x)/x$

TABLE 8.2C (continued)

 $\{(\sin x)/x\} \times 10^4$

| x
radians | $\frac{\sin x}{x}$ | x
radians | $\frac{\sin x}{x}$ | x
radians | $\frac{\sin x}{x}$ | x
radians | $\frac{\sin x}{x}$ | x
radians | $\frac{\sin x}{x}$ |
|----------------|--------------------|----------------|--------------------|----------------|--------------------|----------------|--------------------|----------------|--------------------|
| 57.50 | +142 | 59.75 | -10 | 62.00 | -119 | 64.25 | +154 | 66.50 | -76 |
| .55 | 146 | .80 | 18 | .05 | 114 | .30 | 155 | .55 | 82 |
| .60 | 151 | .85 | 27 | .10 | 108 | .35 | 155 | .60 | 88 |
| .65 | 155 | .90 | 35 | .15 | 101 | .40 | 155 | .65 | 94 |
| .70 | 158 | .95 | 43 | .20 | 95 | .45 | 155 | .70 | 100 |
| 57.75 | +161 | 60.00 | -51 | 62.25 | -88 | 64.50 | +154 | 66.75 | -105 |
| .80 | 164 | .05 | 59 | .30 | 81 | .55 | 153 | .80 | 110 |
| .85 | 167 | .10 | 66 | .35 | 74 | .60 | 152 | .85 | 115 |
| .90 | 169 | .15 | 74 | .40 | 67 | .65 | 150 | .90 | 120 |
| .95 | 170 | .20 | 81 | .45 | 60 | .70 | 148 | .95 | 124 |
| 58.00 | +171 | 60.25 | -88 | 62.50 | -52 | 64.75 | +145 | 67.00 | -128 |
| .05 | 172 | .30 | 95 | .55 | 44 | .80 | 142 | .05 | 131 |
| .10 | 172 | .35 | 102 | .60 | 37 | .85 | 139 | .10 | 135 |
| .15 | 172 | .40 | 108 | .65 | 29 | .90 | 135 | .15 | 137 |
| .20 | 171 | .45 | 114 | .70 | 21 | .95 | 131 | .20 | 140 |
| 58.25 | +170 | 60.50 | -120 | 62.75 | -13 | 65.00 | +127 | 67.25 | -142 |
| .30 | 169 | .55 | 125 | .80 | -5 | .05 | 123 | .30 | 144 |
| .35 | 167 | .60 | 130 | .85 | +3 | .10 | 118 | .35 | 146 |
| .40 | 165 | .65 | 135 | .90 | 11 | .15 | 113 | .40 | 147 |
| .45 | 162 | .70 | 139 | .95 | 19 | .20 | 107 | .45 | 148 |
| 58.50 | +159 | 60.75 | -144 | 63.00 | +27 | 65.25 | +101 | 67.50 | -148 |
| .55 | 155 | .80 | 147 | .05 | 34 | .30 | 96 | .55 | 148 |
| .60 | 151 | .85 | 151 | .10 | 42 | .35 | 89 | .60 | 148 |
| .65 | 147 | .90 | 154 | .15 | 50 | .40 | 83 | .65 | 147 |
| .70 | 142 | .95 | 156 | .20 | 57 | .45 | 76 | .70 | 146 |
| 58.75 | +137 | 61.00 | -158 | 63.25 | +64 | 65.50 | +70 | 67.75 | -144 |
| .80 | 132 | .05 | 160 | .30 | 71 | .55 | 63 | .80 | 143 |
| .85 | 127 | .10 | 162 | .35 | 78 | .60 | 56 | .85 | 141 |
| .90 | 121 | .15 | 163 | .40 | 85 | .65 | 48 | .90 | 138 |
| .95 | 114 | .20 | 163 | .45 | 91 | .70 | 41 | .95 | 135 |
| 59.00 | +108 | 61.25 | -163 | 63.50 | +98 | 65.75 | +34 | 68.00 | -132 |
| .05 | 101 | .30 | 163 | .55 | 104 | .80 | 26 | .05 | 129 |
| .10 | 94 | .35 | 162 | .60 | 109 | .85 | 19 | .10 | 125 |
| .15 | 87 | .40 | 161 | .65 | 115 | .90 | 11 | .15 | 121 |
| .20 | 80 | .45 | 160 | .70 | 120 | .95 | 4 | .20 | 116 |
| 59.25 | +72 | 61.50 | -158 | 63.75 | +125 | 66.00 | -4 | 68.25 | -112 |
| .30 | 64 | .55 | 156 | .80 | 129 | .05 | 12 | .30 | 107 |
| .35 | 56 | .60 | 153 | .85 | 133 | .10 | 19 | .35 | 101 |
| .40 | 48 | .65 | 150 | .90 | 137 | .15 | 27 | .40 | 96 |
| .45 | 40 | .70 | 147 | .95 | 141 | .20 | 34 | .45 | 90 |
| 59.50 | +32 | 61.75 | -143 | 64.00 | +144 | 66.25 | -41 | 68.50 | -84 |
| .55 | 23 | .80 | 139 | .05 | 147 | .30 | 48 | .55 | 78 |
| .60 | 15 | .85 | 134 | .10 | 149 | .35 | 55 | .60 | 72 |
| .65 | +7 | .90 | 130 | .15 | 151 | .40 | 62 | .65 | 65 |
| .70 | -2 | .95 | 125 | .20 | 153 | .45 | 69 | .70 | 59 |

8.2. A FOUR-PLACE TABLE OF $(\sin x)/x$

TABLE 8.2C (continued)

 $\{(\sin x)/x\} \times 10^4$

| x
radians | $\frac{\sin x}{x}$ | x
radians | $\frac{\sin x}{x}$ | x
radians | $\frac{\sin x}{x}$ | x
radians | $\frac{\sin x}{x}$ | x
radians | $\frac{\sin x}{x}$ |
|----------------|--------------------|----------------|--------------------|----------------|--------------------|----------------|--------------------|----------------|--------------------|
| 68.75 | -52 | 71.00 | +134 | 73.25 | -114 | 75.50 | +13 | 77.75 | +91 |
| .80 | 45 | .05 | 132 | .30 | 118 | .55 | 20 | .80 | 87 |
| .85 | 38 | .10 | 129 | .35 | 121 | .60 | 27 | .85 | 82 |
| .90 | 31 | .15 | 126 | .40 | 124 | .65 | 33 | .90 | 77 |
| .95 | 24 | .20 | 122 | .45 | 127 | .70 | 39 | .95 | 71 |
| 69.00 | -17 | 71.25 | +119 | 73.50 | -129 | 75.75 | +45 | 78.00 | +66 |
| .05 | 9 | .30 | 115 | .55 | 131 | .80 | 52 | .05 | 60 |
| .10 | -2 | .35 | 110 | .60 | 132 | .85 | 58 | .10 | 55 |
| .15 | +5 | .40 | 106 | .65 | 134 | .90 | 63 | .15 | 49 |
| .20 | 12 | .45 | 101 | .70 | 135 | .95 | 69 | .20 | 43 |
| 69.25 | +19 | 71.50 | +96 | 73.75 | -135 | 76.00 | +74 | 78.25 | +37 |
| .30 | 27 | .55 | 91 | .80 | 135 | .05 | 80 | .30 | 30 |
| .35 | 34 | .60 | 85 | .85 | 135 | .10 | 85 | .35 | 24 |
| .40 | 41 | .65 | 80 | .90 | 135 | .15 | 90 | .40 | 18 |
| .45 | 47 | .70 | 74 | .95 | 134 | .20 | 94 | .45 | 11 |
| 69.50 | +54 | 71.75 | +68 | 74.00 | -133 | 76.25 | +99 | 78.50 | +5 |
| .55 | 61 | .80 | 61 | .05 | 132 | .30 | 103 | .55 | -1 |
| .60 | 67 | .85 | 55 | .10 | 130 | .35 | 107 | .60 | 8 |
| .65 | 73 | .90 | 49 | .15 | 128 | .40 | 110 | .65 | 14 |
| .70 | 79 | .95 | 42 | .20 | 126 | .45 | 114 | .70 | 20 |
| 69.75 | +85 | 72.00 | +35 | 74.25 | -123 | 76.50 | +117 | 78.75 | -26 |
| .80 | 91 | .05 | 28 | .30 | 120 | .55 | 119 | .80 | 33 |
| .85 | 96 | .10 | 22 | .35 | 117 | .60 | 122 | .85 | 39 |
| .90 | 101 | .15 | 15 | .40 | 113 | .65 | 124 | .90 | 45 |
| .95 | 106 | .20 | 8 | .45 | 109 | .70 | 126 | .95 | 51 |
| 70.00 | +111 | 72.25 | +1 | 74.50 | -105 | 76.75 | +127 | 79.00 | -56 |
| .05 | 115 | .30 | -6 | .55 | 101 | .80 | 128 | .05 | 62 |
| .10 | 119 | .35 | 13 | .60 | 96 | .85 | 129 | .10 | 67 |
| .15 | 123 | .40 | 20 | .65 | 91 | .90 | 130 | .15 | 72 |
| .20 | 126 | .45 | 27 | .70 | 86 | .95 | 130 | .20 | 77 |
| 70.25 | -129 | 72.50 | -33 | 74.75 | -81 | 77.00 | +130 | 79.25 | -82 |
| .30 | 132 | .55 | 40 | .80 | 75 | .05 | 129 | .30 | 87 |
| .35 | 134 | .60 | 46 | .85 | 70 | .10 | 129 | .35 | 91 |
| .40 | 136 | .65 | 53 | .90 | 64 | .15 | 128 | .40 | 95 |
| .45 | 138 | .70 | 59 | .95 | 58 | .20 | 126 | .45 | 99 |
| 70.50 | +139 | 72.75 | -65 | 75.00 | -52 | 77.25 | +124 | 79.50 | -103 |
| .55 | 140 | .80 | 71 | .05 | 45 | .30 | 122 | .55 | 106 |
| .60 | 141 | .85 | 77 | .10 | 39 | .35 | 120 | .60 | 110 |
| .65 | 141 | .90 | 82 | .15 | 33 | .40 | 117 | .65 | 112 |
| .70 | 141 | .95 | 88 | .20 | 26 | .45 | 114 | .70 | 115 |
| 70.75 | +141 | 73.00 | -93 | 75.25 | -20 | 77.50 | +111 | 79.75 | -117 |
| .80 | 140 | .05 | 98 | .30 | 13 | .55 | 108 | .80 | 119 |
| .85 | 139 | .10 | 102 | .35 | -6 | .60 | 104 | .85 | 121 |
| .90 | 138 | .15 | 107 | .40 | +0 | .65 | 100 | .90 | 122 |
| .95 | 136 | .20 | 111 | .45 | 7 | .70 | 96 | .95 | 123 |

8.2. A FOUR-PLACE TABLE OF $(\sin x)/x$

TABLE 8.2C (continued)

 $\{(\sin x)/x\} \times 10^4$

| x
radians | $\frac{\sin x}{x}$ | x
radians | $\frac{\sin x}{x}$ | x
radians | $\frac{\sin x}{x}$ | x
radians | $\frac{\sin x}{x}$ | x
radians | $\frac{\sin x}{x}$ |
|----------------|--------------------|----------------|--------------------|----------------|--------------------|----------------|--------------------|----------------|--------------------|
| 80.00 | -124 | 82.25 | +65 | 84.50 | +38 | 86.75 | -108 | 89.00 | +97 |
| .05 | 125 | .30 | 70 | .55 | 32 | .80 | 106 | .05 | 99 |
| .10 | 125 | .35 | 75 | .60 | 26 | .85 | 103 | .10 | 102 |
| .15 | 125 | .40 | 80 | .65 | 20 | .90 | 101 | .15 | 104 |
| .20 | 124 | .45 | 84 | .70 | 14 | .95 | 98 | .20 | 106 |
| 80.25 | -123 | 82.50 | +89 | 84.75 | +9 | 87.00 | -94 | 89.25 | +108 |
| .30 | 122 | .55 | 92 | .80 | +3 | .05 | 91 | .30 | 109 |
| .35 | 121 | .60 | 96 | .85 | -3 | .10 | 87 | .35 | 110 |
| .40 | 119 | .65 | 100 | .90 | 9 | .15 | 83 | .40 | 111 |
| .45 | 117 | .70 | 103 | .95 | 15 | .20 | 79 | .45 | 111 |
| 80.50 | -115 | 82.75 | +106 | 85.00 | -21 | 87.25 | -75 | 89.50 | +112 |
| .55 | 112 | .80 | 109 | .05 | 26 | .30 | 71 | .55 | 112 |
| .60 | 110 | .85 | 111 | .10 | 32 | .35 | 66 | .60 | 111 |
| .65 | 106 | .90 | 113 | .15 | 38 | .40 | 61 | .65 | 111 |
| .70 | 103 | .95 | 115 | .20 | 43 | .45 | 56 | .70 | 110 |
| 80.75 | -99 | 83.00 | +117 | 85.25 | -49 | 87.50 | -51 | 89.75 | +109 |
| .80 | 95 | .05 | 118 | .30 | 54 | .55 | 46 | .80 | 107 |
| .85 | 91 | .10 | 119 | .35 | 59 | .60 | 41 | .85 | 106 |
| .90 | 87 | .15 | 120 | .40 | 64 | .65 | 35 | .90 | 104 |
| .95 | 83 | .20 | 120 | .45 | 69 | .70 | 30 | .95 | 102 |
| 81.00 | -78 | 83.25 | +120 | 85.50 | -73 | 87.75 | -24 | 90.00 | +99 |
| .05 | 72 | .30 | 120 | .55 | 78 | .80 | 19 | .05 | 97 |
| .10 | 68 | .35 | 119 | .60 | 82 | .85 | 13 | .10 | 94 |
| .15 | 62 | .40 | 119 | .65 | 86 | .90 | 7 | .15 | 91 |
| .20 | 57 | .45 | 117 | .70 | 90 | .95 | 2 | .20 | 87 |
| 81.25 | -51 | 83.50 | +116 | 85.75 | -93 | 88.00 | +4 | 90.25 | +84 |
| .30 | 46 | .55 | 114 | .80 | 97 | .05 | 10 | .30 | 80 |
| .35 | 41 | .60 | 112 | .85 | 100 | .10 | 15 | .35 | 76 |
| .40 | 34 | .65 | 110 | .90 | 103 | .15 | 21 | .40 | 72 |
| .45 | 28 | .70 | 108 | .95 | 105 | .20 | 26 | .45 | 67 |
| 81.50 | -22 | 83.75 | +105 | 86.00 | -107 | 88.25 | +32 | 90.50 | +63 |
| .55 | 16 | .80 | 102 | .05 | 109 | .30 | 37 | .55 | 58 |
| .60 | 10 | .85 | 99 | .10 | 111 | .35 | 43 | .60 | 54 |
| .65 | -4 | .90 | 95 | .15 | 113 | .40 | 48 | .65 | 49 |
| .70 | +2 | .95 | 91 | .20 | 114 | .45 | 53 | .70 | 44 |
| 81.75 | +8 | 84.00 | +87 | 86.25 | -115 | 88.50 | +58 | 90.75 | +38 |
| .80 | 14 | .05 | 83 | .30 | 115 | .55 | 62 | .80 | 33 |
| .85 | 21 | .10 | 79 | .35 | 116 | .60 | 67 | .85 | 28 |
| .90 | 26 | .15 | 74 | .40 | 116 | .65 | 71 | .90 | 23 |
| .95 | 32 | .20 | 69 | .45 | 115 | .70 | 76 | .95 | 17 |
| 82.00 | +38 | 84.25 | +64 | 86.50 | -115 | 88.75 | +80 | 91.00 | +12 |
| .05 | 44 | .30 | 59 | .55 | 114 | .80 | 84 | .05 | 6 |
| .10 | 50 | .35 | 54 | .60 | 113 | .85 | 87 | .10 | +1 |
| .15 | 55 | .40 | 49 | .65 | 112 | .90 | 91 | .15 | -5 |
| .20 | 60 | .45 | 43 | .70 | 110 | .95 | 94 | .20 | 10 |

8.2. A FOUR-PLACE TABLE OF $(\sin x)/x$

TABLE 8.2C (continued)

 $\{(\sin x)/x\} \times 10^4$

| x
radians | $\frac{\sin x}{x}$ | x
radians | $\frac{\sin x}{x}$ | x
radians | $\frac{\sin x}{x}$ | x
radians | $\frac{\sin x}{x}$ | x
radians | $\frac{\sin x}{x}$ |
|----------------|--------------------|----------------|--------------------|----------------|--------------------|----------------|--------------------|----------------|--------------------|
| 91.25 | -16 | 93.00 | -102 | 94.75 | +51 | 96.50 | +80 | 98.25 | -77 |
| .30 | 21 | .05 | 100 | .80 | 55 | .55 | 77 | .30 | 80 |
| .35 | 26 | .10 | 98 | .85 | 60 | .60 | 73 | .35 | 83 |
| .40 | 32 | .15 | 96 | .90 | 64 | .65 | 70 | .40 | 86 |
| .45 | 37 | .20 | 93 | .95 | 68 | .70 | 66 | .45 | 89 |
| 91.50 | -42 | 93.25 | -90 | 95.00 | +72 | 96.75 | +62 | 98.50 | -91 |
| .55 | 47 | .30 | 87 | .05 | 76 | .80 | 57 | .55 | 93 |
| .60 | 52 | .35 | 84 | .10 | 79 | .85 | 53 | .60 | 95 |
| .65 | 56 | .40 | 80 | .15 | 82 | .90 | 49 | .65 | 97 |
| .70 | 61 | .45 | 77 | .20 | 86 | .95 | 44 | .70 | 98 |
| 91.75 | -65 | 93.50 | -73 | 95.25 | +88 | 97.00 | +39 | 98.75 | -99 |
| .80 | 70 | .55 | 69 | .30 | 91 | .05 | 34 | .80 | 100 |
| .85 | 74 | .60 | 64 | .35 | 94 | .10 | 29 | .85 | 101 |
| .90 | 78 | .65 | 60 | .40 | 96 | .15 | 24 | .90 | 101 |
| .95 | 81 | .70 | 56 | .45 | 98 | .20 | 19 | .95 | 101 |
| 92.00 | -85 | 93.75 | -51 | 95.50 | +99 | 97.25 | +14 | 99.00 | -101 |
| .05 | 88 | .80 | 46 | .55 | 101 | .30 | 9 | .05 | 101 |
| .10 | 91 | .85 | 41 | .60 | 102 | .35 | +4 | .10 | 100 |
| .15 | 94 | .90 | 36 | .65 | 103 | .40 | -1 | .15 | 99 |
| .20 | 96 | .95 | 31 | .70 | 104 | .45 | 6 | .20 | 98 |
| 92.25 | -99 | 94.00 | -26 | 95.75 | +104 | 97.50 | -11 | 99.25 | -97 |
| .30 | 101 | .05 | 21 | .80 | 104 | .55 | 16 | .30 | 95 |
| .35 | 103 | .10 | 16 | .85 | 104 | .60 | 21 | .35 | 93 |
| .40 | 104 | .15 | 10 | .90 | 104 | .65 | 26 | .40 | 91 |
| .45 | 105 | .20 | 5 | .95 | 103 | .70 | 31 | .45 | 89 |
| 92.50 | -106 | 94.25 | +0 | 96.00 | +102 | 97.75 | -36 | 99.50 | -86 |
| .55 | 107 | .30 | 6 | .05 | 101 | .80 | 41 | .55 | 83 |
| .60 | 108 | .35 | 11 | .10 | 100 | .85 | 45 | .60 | 81 |
| .65 | 108 | .40 | 16 | .15 | 98 | .90 | 50 | .65 | 77 |
| .70 | 108 | .45 | 21 | .20 | 96 | .95 | 54 | .70 | 74 |
| 92.75 | -108 | 94.50 | +26 | 96.25 | +94 | 98.00 | -59 | 99.75 | -71 |
| .80 | 107 | .55 | 31 | .30 | 92 | .05 | 63 | .80 | 67 |
| .85 | 106 | .60 | 36 | .35 | 89 | .10 | 66 | .85 | 63 |
| .90 | 105 | .65 | 41 | .40 | 87 | .15 | 70 | .90 | 59 |
| .95 | 104 | .70 | 46 | .45 | 84 | .20 | 74 | .95 | 55 |
| | | | | | | | | 100.00 | -51 |

8.3. A Short Table of $\sin 2\pi x$; $\cos 2\pi x$

TABLE 8.3
 $\sin 2\pi x$; $\cos 2\pi x$ (x fractional)

| $\sin 2\pi x$
—
+
x | $\cos 2\pi x$
—
+
x | $\sin 2\pi x$
+
—
x | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|--------------------------------|--------------------------------|--------------------------------|--------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----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| $\cdot 75$ $\cdot 25$ | $\cdot 50$ $\cdot 00$ | 1·0000 | 1·0000 | ·001 | ·002 | ·003 | ·004 | ·005 | ·006 | ·007 | ·008 | ·009 | 9980 | 9984 | 9987 | 9990 | 9993 | 9995 | 9997 | 9998 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 | 9999 |

TABLE 8.4 Table of Product

| | | | | | | | | | | | | |
|---|-----|----|----|----|----|----|----|----|----|----|----|----|
| + | ·75 | 76 | 77 | 78 | 79 | 80 | 81 | 82 | 83 | 84 | 85 | 86 |
| − | ·75 | 74 | 73 | 72 | 71 | 70 | 69 | 68 | 67 | 66 | 65 | 64 |
| − | ·25 | 26 | 27 | 28 | 29 | 30 | 31 | 32 | 33 | 34 | 35 | 36 |
| + | ·25 | 24 | 23 | 22 | 21 | 20 | 19 | 18 | 17 | 16 | 15 | 14 |

| | | | | | 000 | 063 | 125 | 187 | 249 | 309 | 368 | 426 | 482 | 536 | 588 | 637 | 6 |
|---------------|------|-----|-----|-----|------|-----|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| y for cosines | ·75 | ·75 | ·25 | ·25 | 000 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| | 76 | 74 | 26 | 24 | 063 | 0 | ·004 | 008 | 012 | 016 | 019 | 023 | 027 | 030 | 034 | 037 | 040 |
| | 77 | 73 | 27 | 23 | 125 | 0 | ·008 | 016 | 023 | 031 | 039 | 046 | 053 | 060 | 067 | 073 | 080 |
| | 78 | 72 | 28 | 22 | 187 | 0 | ·012 | 023 | 035 | 047 | 058 | 069 | 080 | 090 | 100 | 110 | 119 |
| | 79 | 71 | 29 | 21 | 249 | 0 | ·016 | 031 | 047 | 062 | 077 | 092 | 106 | 120 | 133 | 146 | 159 |
| | 80 | 70 | 30 | 20 | 309 | 0 | ·019 | 039 | 058 | 077 | 095 | 114 | 132 | 149 | 166 | 182 | 197 |
| | 81 | 69 | 31 | 19 | 368 | 0 | ·023 | 046 | 069 | 092 | 114 | 135 | 158 | 177 | 197 | 216 | 234 |
| | 82 | 68 | 32 | 18 | 426 | 0 | ·027 | 053 | 080 | 106 | 132 | 158 | 181 | 205 | 228 | 250 | 271 |
| | 83 | 67 | 33 | 17 | 482 | 0 | ·030 | 060 | 090 | 120 | 149 | 177 | 205 | 232 | 258 | 283 | 307 |
| | 84 | 66 | 34 | 16 | 536 | 0 | ·034 | 067 | 100 | 133 | 166 | 197 | 228 | 258 | 287 | 315 | 341 |
| | 85 | 65 | 35 | 15 | 588 | 0 | ·037 | 073 | 110 | 146 | 182 | 216 | 250 | 283 | 315 | 346 | 375 |
| | 86 | 64 | 36 | 14 | 637 | 0 | ·040 | 080 | 119 | 159 | 197 | 234 | 271 | 307 | 341 | 375 | 406 |
| | 87 | 63 | 37 | 13 | 684 | 0 | ·043 | 086 | 128 | 170 | 211 | 252 | 291 | 330 | 367 | 402 | 436 |
| | 88 | 62 | 38 | 12 | 729 | 0 | ·046 | 091 | 136 | 182 | 225 | 268 | 310 | 351 | 391 | 429 | 464 |
| | 89 | 61 | 39 | 11 | 770 | 0 | ·048 | 096 | 144 | 192 | 238 | 283 | 328 | 361 | 413 | 453 | 490 |
| | 90 | 60 | 40 | 10 | 809 | 0 | ·051 | 101 | 151 | 201 | 250 | 298 | 345 | 390 | 434 | 476 | 515 |
| | 91 | 59 | 41 | 09 | 844 | 0 | ·053 | 106 | 158 | 210 | 261 | 311 | 360 | 407 | 452 | 496 | 538 |
| | 92 | 58 | 42 | 08 | 876 | 0 | ·055 | 110 | 164 | 218 | 271 | 322 | 373 | 422 | 470 | 515 | 558 |
| | 93 | 57 | 43 | 07 | 905 | 0 | ·057 | 113 | 170 | 225 | 280 | 333 | 386 | 436 | 485 | 532 | 576 |
| | 94 | 56 | 44 | 06 | 930 | 0 | ·059 | 116 | 174 | 232 | 287 | 342 | 396 | 448 | 498 | 547 | 592 |
| | 95 | 55 | 45 | 05 | 951 | 0 | ·060 | 119 | 178 | 237 | 294 | 350 | 405 | 458 | 510 | 559 | 606 |
| | 96 | 54 | 46 | 04 | 969 | 0 | ·061 | 121 | 181 | 241 | 300 | 357 | 413 | 467 | 519 | 570 | 617 |
| | 97 | 53 | 47 | 03 | 982 | 0 | ·062 | 123 | 184 | 245 | 304 | 361 | 418 | 473 | 526 | 577 | 626 |
| | 98 | 52 | 48 | 02 | 992 | 0 | ·062 | 124 | 186 | 247 | 307 | 365 | 423 | 478 | 532 | 583 | 632 |
| | 99 | 51 | 49 | 01 | 998 | 0 | ·062 | 125 | 187 | 249 | 308 | 367 | 425 | 481 | 535 | 587 | 636 |
| | 1·00 | 50 | 50 | 00 | 1·00 | 0 | ·063 | 125 | 187 | 249 | 309 | 368 | 426 | 482 | 536 | 588 | 637 |

| | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|------|-----|----|----|----|----|----|----|----|----|----|----|----|
| + | − | − | + | | + | ·00 | 01 | 02 | 03 | 04 | 05 | 06 | 07 | 08 | 09 | 10 | 11 |
| | | | | + | ·50 | 49 | 48 | 47 | 46 | 45 | 44 | 43 | 42 | 41 | 40 | 39 | |
| | | | | − | ·50 | 51 | 52 | 53 | 54 | 55 | 56 | 57 | 58 | 59 | 60 | 61 | |
| | | | | − | 1·00 | 99 | 98 | 97 | 96 | 95 | 94 | 93 | 92 | 91 | 90 | 89 | |

Products

$2\pi x \left\{ \frac{\cos}{\sin} \right\} 2\pi y \quad (x, y \text{ fractional})$

ies

| | | | | | | | | | | | | |
|----|----|----|----|----|----|----|----|----|----|----|------|---|
| 89 | 90 | 91 | 92 | 93 | 94 | 95 | 96 | 97 | 98 | 99 | 1.00 | + |
| 61 | 60 | 59 | 58 | 57 | 56 | 55 | 54 | 53 | 52 | 51 | 50 | — |
| 39 | 40 | 41 | 42 | 43 | 44 | 45 | 46 | 47 | 48 | 49 | 50 | — |
| 11 | 10 | 09 | 08 | 07 | 06 | 05 | 04 | 03 | 02 | 01 | 0 | + |

| 770 | 809 | 844 | 876 | 905 | 930 | 951 | 969 | 982 | 992 | 998 | 1.00 | + | + | — | — |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|-----|-----|-----|------|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | .00 | .50 | .50 | 1.00 |
| 048 | 051 | 053 | 055 | 057 | 059 | 060 | 061 | 062 | 062 | 062 | 063 | 01 | 49 | 51 | 99 |
| 096 | 101 | 106 | 110 | 113 | 116 | 119 | 121 | 123 | 124 | 125 | 125 | 02 | 48 | 52 | 98 |
| 144 | 151 | 158 | 164 | 170 | 174 | 178 | 181 | 184 | 186 | 187 | 187 | 03 | 47 | 53 | 97 |
| 192 | 201 | 210 | 218 | 225 | 232 | 237 | 241 | 245 | 247 | 249 | 249 | 04 | 46 | 54 | 96 |
| 238 | 250 | 261 | 271 | 280 | 287 | 294 | 300 | 304 | 307 | 308 | 309 | 05 | 45 | 55 | 95 |
| 283 | 298 | 311 | 322 | 333 | 342 | 350 | 357 | 361 | 365 | 367 | 368 | 06 | 44 | 56 | 94 |
| 328 | 345 | 360 | 373 | 386 | 396 | 405 | 413 | 418 | 423 | 425 | 426 | 07 | 43 | 57 | 93 |
| 371 | 390 | 407 | 422 | 436 | 448 | 458 | 467 | 473 | 478 | 481 | 482 | 08 | 42 | 58 | 92 |
| 413 | 434 | 452 | 470 | 485 | 498 | 510 | 519 | 526 | 532 | 535 | 536 | 09 | 41 | 59 | 91 |
| 453 | 476 | 496 | 515 | 532 | 547 | 559 | 570 | 577 | 583 | 587 | 588 | 10 | 40 | 60 | 90 |
| 490 | 515 | 538 | 558 | 576 | 592 | 606 | 617 | 626 | 632 | 636 | 637 | 11 | 39 | 61 | 89 |
| 527 | 553 | 577 | 599 | 619 | 636 | 650 | 663 | 672 | 679 | 683 | 684 | 12 | 38 | 62 | 88 |
| 561 | 590 | 615 | 639 | 660 | 678 | 693 | 706 | 716 | 723 | 728 | 729 | 13 | 37 | 63 | 87 |
| 593 | 623 | 650 | 675 | 697 | 716 | 732 | 746 | 756 | 764 | 768 | 770 | 14 | 36 | 64 | 86 |
| 623 | 654 | 683 | 709 | 732 | 753 | 769 | 784 | 794 | 803 | 807 | 809 | 15 | 35 | 65 | 85 |
| 650 | 683 | 712 | 739 | 764 | 785 | 803 | 818 | 829 | 837 | 842 | 844 | 16 | 34 | 66 | 84 |
| 675 | 709 | 739 | 767 | 793 | 815 | 833 | 849 | 860 | 869 | 874 | 876 | 17 | 33 | 67 | 83 |
| 697 | 732 | 764 | 793 | 819 | 847 | 861 | 877 | 889 | 898 | 903 | 905 | 18 | 32 | 68 | 82 |
| 716 | 753 | 785 | 815 | 847 | 865 | 884 | 901 | 913 | 923 | 928 | 930 | 19 | 31 | 69 | 81 |
| 732 | 769 | 803 | 833 | 861 | 884 | 904 | 922 | 934 | 943 | 949 | 951 | 20 | 30 | 70 | 80 |
| 746 | 784 | 818 | 849 | 877 | 901 | 922 | 939 | 952 | 961 | 967 | 969 | 21 | 29 | 71 | 79 |
| 756 | 794 | 829 | 860 | 889 | 913 | 934 | 952 | 964 | 974 | 980 | 982 | 22 | 28 | 72 | 78 |
| 764 | 803 | 837 | 869 | 898 | 923 | 943 | 961 | 974 | 984 | 990 | 992 | 23 | 27 | 73 | 77 |
| 768 | 807 | 842 | 874 | 903 | 928 | 949 | 967 | 980 | 990 | 996 | 998 | 24 | 26 | 74 | 76 |
| 770 | 809 | 844 | 876 | 905 | 930 | 951 | 969 | 982 | 992 | 998 | 1.00 | 25 | 25 | 75 | 75 |

y for sines

| | | | | | | | | | | | | | | | |
|----|----|----|----|----|----|----|----|----|----|----|----|---|---|---|---|
| | | | | | | | | | | | | + | + | — | — |
| 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | + | | | |
| 36 | 35 | 34 | 33 | 32 | 31 | 30 | 29 | 28 | 27 | 26 | 25 | + | | | |
| 64 | 65 | 66 | 67 | 68 | 69 | 70 | 71 | 72 | 73 | 74 | 75 | — | | | |
| 86 | 85 | 84 | 83 | 82 | 81 | 80 | 79 | 78 | 77 | 76 | 75 | — | | | |

TABLE 8.5A
 $\sin 2\pi hx$ (h odd) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=1$ | 3 | 5 | 7 | 9 | 11 | 13 | 15 | 17 | 19 | Change sign.
x | |
|-----------------------|-----|-------|-----|-----|------|------|------|------|------|------|------|---------------------|------|
| 000 | 500 | 000 | 000 | 000 | 000 | 000 | 000 | 000 | 000 | 000 | 000 | 500 | 1000 |
| 001 | 499 | 006 | 019 | 031 | 044 | 057 | 069 | 082 | 094 | 107 | 119 | 501 | 999 |
| 002 | 498 | 013 | 038 | 063 | 088 | 113 | 138 | 163 | 187 | 212 | 237 | 502 | 998 |
| 003 | 497 | 019 | 057 | 094 | 132 | 169 | 206 | 243 | 279 | 315 | 351 | 503 | 997 |
| 004 | 496 | 025 | 075 | 125 | 175 | 224 | 273 | 321 | 368 | 414 | 460 | 504 | 996 |
| | | | | | | | | | | | | | |
| 005 | 495 | 031 | 094 | 156 | 218 | 279 | 339 | 397 | 454 | 509 | 562 | 505 | 995 |
| 006 | 494 | 038 | 113 | 187 | 261 | 333 | 403 | 471 | 536 | 598 | 657 | 506 | 994 |
| 007 | 493 | 044 | 132 | 218 | 303 | 386 | 465 | 541 | 613 | 680 | 742 | 507 | 993 |
| 008 | 492 | 050 | 150 | 249 | 345 | 437 | 525 | 608 | 685 | 754 | 816 | 508 | 992 |
| 009 | 491 | 057 | 169 | 279 | 386 | 487 | 583 | 671 | 750 | 820 | 879 | 509 | 991 |
| | | | | | | | | | | | | | |
| 010 | 490 | 063 | 187 | 309 | 426 | 536 | 637 | 729 | 809 | 876 | 930 | 510 | 990 |
| 011 | 489 | 069 | 206 | 339 | 465 | 583 | 689 | 782 | 861 | 923 | 967 | 511 | 989 |
| 012 | 488 | 075 | 224 | 368 | 504 | 628 | 738 | 831 | 905 | 959 | 990 | 512 | 988 |
| 013 | 487 | 082 | 243 | 397 | 541 | 671 | 782 | 873 | 941 | 983 | 1000 | 513 | 987 |
| 014 | 486 | 088 | 261 | 426 | 578 | 712 | 824 | 910 | 969 | 997 | 995 | 514 | 986 |
| | | | | | | | | | | | | | |
| 015 | 485 | 094 | 279 | 454 | 613 | 750 | 861 | 941 | 988 | 1000 | 976 | 515 | 985 |
| 016 | 484 | 100 | 297 | 482 | 647 | 786 | 894 | 965 | 998 | 990 | 943 | 516 | 984 |
| 017 | 483 | 107 | 315 | 509 | 680 | 820 | 923 | 983 | 1000 | 970 | 897 | 517 | 983 |
| 018 | 482 | 113 | 333 | 536 | 712 | 851 | 947 | 995 | 992 | 939 | 838 | 518 | 982 |
| 019 | 481 | 119 | 351 | 562 | 742 | 879 | 967 | 1000 | 976 | 897 | 767 | 519 | 981 |
| | | | | | | | | | | | | | |
| 020 | 480 | 125 | 368 | 588 | 771 | 905 | 982 | 998 | 951 | 844 | 685 | 520 | 980 |
| 021 | 479 | 132 | 386 | 613 | 798 | 927 | 993 | 990 | 918 | 782 | 593 | 521 | 979 |
| 022 | 478 | 138 | 403 | 637 | 824 | 947 | 999 | 975 | 876 | 712 | 493 | 522 | 978 |
| 023 | 477 | 144 | 420 | 661 | 848 | 964 | 1000 | 953 | 827 | 633 | 386 | 523 | 977 |
| 024 | 476 | 150 | 437 | 685 | 870 | 977 | 996 | 925 | 771 | 546 | 273 | 524 | 976 |
| | | | | | | | | | | | | | |
| 025 | 475 | 156 | 454 | 707 | 891 | 988 | 988 | 891 | 707 | 454 | 156 | 525 | 975 |
| 026 | 474 | 163 | 471 | 729 | 910 | 995 | 975 | 851 | 637 | 356 | 038 | 526 | 974 |
| 027 | 473 | 169 | 487 | 750 | 927 | 999 | 957 | 805 | 562 | 255 | -082 | 527 | 973 |
| 028 | 472 | 175 | 504 | 771 | 943 | 1000 | 934 | 754 | 482 | 150 | -200 | 528 | 972 |
| 029 | 471 | 181 | 520 | 790 | 957 | 998 | 907 | 698 | 397 | 044 | -315 | 529 | 971 |
| | | | | | | | | | | | | | |
| 030 | 470 | 187 | 536 | 809 | 969 | 992 | 876 | 637 | 309 | -063 | -426 | 530 | 970 |
| 031 | 469 | 194 | 552 | 827 | 979 | 983 | 841 | 572 | 218 | -169 | -531 | 531 | 969 |
| 032 | 468 | 200 | 567 | 844 | 987 | 972 | 802 | 504 | 125 | -273 | -628 | 532 | 968 |
| 033 | 467 | 206 | 583 | 861 | 993 | 957 | 758 | 431 | 031 | -374 | -716 | 533 | 967 |
| 034 | 466 | 212 | 598 | 876 | 997 | 939 | 712 | 356 | -063 | -471 | -794 | 534 | 966 |
| | | | | | | | | | | | | | |
| 035 | 465 | 218 | 613 | 891 | 1000 | 918 | 661 | 279 | -156 | -562 | -861 | 535 | 965 |
| 036 | 464 | 224 | 628 | 905 | 1000 | 894 | 608 | 200 | -249 | -647 | -915 | 536 | 964 |
| 037 | 463 | 230 | 642 | 918 | 998 | 867 | 552 | 119 | -339 | -725 | -957 | 537 | 963 |
| 038 | 462 | 237 | 657 | 930 | 995 | 838 | 493 | 038 | -426 | -794 | -985 | 538 | 962 |
| 039 | 461 | 243 | 671 | 941 | 990 | 805 | 431 | -044 | -509 | -854 | -998 | 539 | 961 |

TABLE 8.5A
 $\sin 2\pi hx$ (h odd) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=21$ | 23 | 25 | 27 | 29 | 31 | 33 | 35 | 37 | 39 | Change sign.
x | |
|-----------------------|-----|--------|------|-------|------|-------|------|------|------|------|------|---------------------|------|
| 000 | 500 | 000 | 000 | 000 | 000 | 000 | 000 | 000 | 000 | 000 | 000 | 500 | 1000 |
| 001 | 499 | 132 | 144 | 156 | 169 | 181 | 194 | 206 | 218 | 230 | 243 | 501 | 999 |
| 002 | 498 | 261 | 285 | 309 | 333 | 356 | 380 | 403 | 426 | 448 | 471 | 502 | 998 |
| 003 | 497 | 386 | 420 | 454 | 487 | 520 | 552 | 583 | 613 | 642 | 671 | 503 | 997 |
| 004 | 496 | 504 | 546 | 588 | 628 | 666 | 703 | 738 | 771 | 802 | 831 | 504 | 996 |
| | | | | | | | | | | | | | |
| 005 | 495 | 613 | 661 | 707 | 750 | 790 | 827 | 861 | 891 | 918 | 941 | 505 | 995 |
| 006 | 494 | 712 | 762 | 809 | 851 | 888 | 920 | 947 | 969 | 985 | 995 | 506 | 994 |
| 007 | 493 | 798 | 848 | 891 | 927 | 957 | 979 | 993 | 1000 | 998 | 990 | 507 | 993 |
| 008 | 492 | 870 | 915 | 951 | 977 | 994 | 1000 | 996 | 982 | 959 | 925 | 508 | 992 |
| 009 | 491 | 927 | 964 | 988 | 999 | 998 | 983 | 957 | 918 | 867 | 805 | 509 | 991 |
| | | | | | | | | | | | | | |
| 010 | 490 | 969 | 992 | 1000 | 992 | 969 | 930 | 876 | 809 | 729 | 637 | 510 | 990 |
| 011 | 489 | 993 | 1000 | 988 | 957 | 907 | 841 | 758 | 661 | 552 | 431 | 511 | 989 |
| 012 | 488 | 1000 | 987 | 951 | 894 | 816 | 720 | 608 | 482 | 345 | 200 | 512 | 988 |
| 013 | 487 | 990 | 953 | 891 | 805 | 698 | 572 | 431 | 279 | 119 | -044 | 513 | 987 |
| 014 | 486 | 962 | 899 | 809 | 694 | 557 | 403 | 237 | 063 | -113 | -285 | 514 | 986 |
| | | | | | | | | | | | | | |
| 015 | 485 | 918 | 827 | 707 | 562 | 397 | 218 | 031 | -156 | -339 | -509 | 515 | 985 |
| 016 | 484 | 858 | 738 | 588 | 414 | 224 | 025 | -175 | -368 | -546 | -703 | 516 | 984 |
| 017 | 483 | 782 | 633 | 454 | 255 | 044 | -169 | -374 | -562 | -725 | -854 | 517 | 983 |
| 018 | 482 | 694 | 514 | 309 | 088 | -138 | -356 | -557 | -729 | -864 | -955 | 518 | 982 |
| 019 | 481 | 593 | 386 | 156 | -082 | -315 | -531 | -716 | -861 | -957 | -998 | 519 | 981 |
| | | | | | | | | | | | | | |
| 020 | 480 | 482 | 249 | 000 | -249 | -482 | -685 | -844 | -951 | -998 | -982 | 520 | 980 |
| 021 | 479 | 362 | 107 | -156 | -409 | -633 | -813 | -937 | -996 | -986 | -907 | 521 | 979 |
| 022 | 478 | 237 | -038 | -309 | -557 | -762 | -910 | -989 | -992 | -920 | -778 | 522 | 978 |
| 023 | 477 | 107 | -181 | -454 | -689 | -867 | -973 | -998 | -941 | -805 | -603 | 523 | 977 |
| 024 | 476 | -025 | -321 | -588 | -802 | -943 | -999 | -965 | -844 | -647 | -391 | 524 | 976 |
| | | | | | | | | | | | | | |
| 025 | 475 | -156 | -454 | -707 | -891 | -988 | -988 | -891 | -707 | -454 | -156 | 525 | 975 |
| 026 | 474 | -285 | -578 | -809 | -955 | -1000 | -939 | -778 | -536 | -237 | 088 | 526 | 974 |
| 027 | 473 | -409 | -689 | -891 | -991 | -979 | -854 | -633 | -339 | -006 | 327 | 527 | 973 |
| 028 | 472 | -525 | -786 | -951 | -999 | -925 | -738 | -460 | -125 | 224 | 546 | 528 | 972 |
| 029 | 471 | -633 | -867 | -988 | -979 | -841 | -593 | -267 | 094 | 443 | 733 | 529 | 971 |
| | | | | | | | | | | | | | |
| 030 | 470 | -729 | -930 | -1000 | -930 | -729 | -426 | -063 | 309 | 637 | 876 | 530 | 970 |
| 031 | 469 | -813 | -973 | -988 | -854 | -593 | -243 | 144 | 509 | 798 | 967 | 531 | 969 |
| 032 | 468 | -882 | -996 | -951 | -754 | -437 | -050 | 345 | 685 | 915 | 1000 | 532 | 968 |
| 033 | 467 | -937 | -998 | -891 | -633 | -267 | 144 | 531 | 827 | 983 | 973 | 533 | 967 |
| 034 | 466 | -975 | -980 | -809 | -493 | -088 | 333 | 694 | 930 | 999 | 888 | 534 | 966 |
| | | | | | | | | | | | | | |
| 035 | 465 | -996 | -941 | -707 | -339 | 094 | 509 | 827 | 988 | 960 | 750 | 535 | 965 |
| 036 | 464 | -999 | -882 | -588 | -175 | 273 | 666 | 925 | 998 | 870 | 567 | 536 | 964 |
| 037 | 463 | -986 | -805 | -454 | -006 | 443 | 798 | 983 | 960 | 733 | 351 | 537 | 963 |
| 038 | 462 | -955 | -712 | -309 | 163 | 598 | 899 | 1000 | 876 | 557 | 113 | 538 | 962 |
| 039 | 461 | -907 | -603 | -156 | 327 | 733 | 967 | 973 | 750 | 351 | -132 | 539 | 961 |

TABLE 8.5A (continued)

 $\sin 2\pi hx$ (h odd) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=1$ | 3 | 5 | 7 | 9 | 11 | 13 | 15 | 17 | 19 | Change sign.
x | |
|-----------------------|-----|-------|------|------|------|-------|-------|-------|-------|-------|------|---------------------|-----|
| 040 | 460 | 249 | 685 | 951 | 982 | 771 | 368 | -125 | -588 | -905 | -998 | 540 | 960 |
| 041 | 459 | 255 | 698 | 960 | 973 | 733 | 303 | -206 | -661 | -945 | -983 | 541 | 959 |
| 042 | 458 | 261 | 712 | 969 | 962 | 694 | 237 | -285 | -729 | -975 | -955 | 542 | 958 |
| 043 | 457 | 267 | 725 | 976 | 949 | 652 | 169 | -362 | -790 | -993 | -913 | 543 | 957 |
| 044 | 456 | 273 | 738 | 982 | 934 | 608 | 100 | -437 | -844 | -1000 | -858 | 544 | 956 |
| 045 | 455 | 279 | 750 | 988 | 918 | 562 | 031 | -509 | -891 | -996 | -790 | 545 | 955 |
| 046 | 454 | 285 | 762 | 992 | 899 | 514 | -038 | -578 | -930 | -980 | -712 | 546 | 954 |
| 047 | 453 | 291 | 775 | 996 | 879 | 465 | -107 | -642 | -960 | -953 | -623 | 547 | 953 |
| 048 | 452 | 297 | 786 | 998 | 858 | 414 | -175 | -703 | -982 | -915 | -525 | 548 | 952 |
| 049 | 451 | 303 | 798 | 1000 | 834 | 362 | -243 | -758 | -996 | -867 | -420 | 549 | 951 |
| 050 | 450 | 309 | 809 | 1000 | 809 | 309 | -309 | -809 | -1000 | -809 | -309 | 550 | 950 |
| 051 | 449 | 315 | 820 | 1000 | 782 | 255 | -374 | -854 | -996 | -742 | -194 | 551 | 949 |
| 052 | 448 | 321 | 831 | 998 | 754 | 200 | -437 | -894 | -982 | -666 | -075 | 552 | 948 |
| 053 | 447 | 327 | 841 | 996 | 725 | 144 | -498 | -927 | -960 | -583 | 044 | 553 | 947 |
| 054 | 446 | 333 | 851 | 992 | 694 | 088 | -557 | -955 | -930 | -493 | 163 | 554 | 946 |
| 055 | 445 | 339 | 861 | 988 | 661 | 031 | -613 | -976 | -891 | -397 | 279 | 555 | 945 |
| 056 | 444 | 345 | 870 | 982 | 628 | -025 | -666 | -990 | -844 | -297 | 391 | 556 | 944 |
| 057 | 443 | 351 | 879 | 976 | 593 | -082 | -716 | -998 | -790 | -194 | 498 | 557 | 943 |
| 058 | 442 | 356 | 888 | 969 | 557 | -138 | -762 | -1000 | -729 | -088 | 598 | 558 | 942 |
| 059 | 441 | 362 | 897 | 960 | 520 | -194 | -805 | -994 | -661 | 019 | 689 | 559 | 941 |
| 060 | 440 | 368 | 905 | 951 | 482 | -249 | -844 | -982 | -588 | 125 | 771 | 560 | 940 |
| 061 | 439 | 374 | 913 | 941 | 443 | -303 | -879 | -964 | -509 | 230 | 841 | 561 | 939 |
| 062 | 438 | 380 | 920 | 930 | 403 | -356 | -910 | -939 | -426 | 333 | 899 | 562 | 938 |
| 063 | 437 | 386 | 927 | 918 | 362 | -409 | -937 | -907 | -339 | 431 | 945 | 563 | 937 |
| 064 | 436 | 391 | 934 | 905 | 321 | -460 | -959 | -870 | -249 | 525 | 977 | 564 | 936 |
| 065 | 435 | 397 | 941 | 891 | 279 | -509 | -976 | -827 | -156 | 613 | 996 | 565 | 935 |
| 066 | 434 | 403 | 947 | 876 | 237 | -557 | -989 | -778 | -063 | 694 | 1000 | 566 | 934 |
| 067 | 433 | 409 | 953 | 861 | 194 | -603 | -997 | -725 | 031 | 767 | 990 | 567 | 933 |
| 068 | 432 | 414 | 959 | 844 | 150 | -647 | -1000 | -666 | 125 | 831 | 965 | 568 | 932 |
| 069 | 431 | 420 | 964 | 827 | 107 | -689 | -998 | -603 | 218 | 885 | 927 | 569 | 931 |
| 070 | 430 | 426 | 969 | 809 | 063 | -729 | -992 | -536 | 309 | 930 | 876 | 570 | 930 |
| 071 | 429 | 431 | 973 | 790 | 019 | -767 | -981 | -465 | 397 | 964 | 813 | 571 | 929 |
| 072 | 428 | 437 | 977 | 771 | -025 | -802 | -965 | -391 | 482 | 987 | 738 | 572 | 928 |
| 073 | 427 | 443 | 981 | 750 | -069 | -834 | -945 | -315 | 562 | 998 | 652 | 573 | 927 |
| 074 | 426 | 448 | 985 | 729 | -113 | -864 | -920 | -237 | 637 | 999 | 557 | 574 | 926 |
| 075 | 425 | 454 | 988 | 707 | -156 | -891 | -891 | -156 | 707 | 988 | 454 | 575 | 925 |
| 076 | 424 | 460 | 990 | 685 | -200 | -915 | -858 | -075 | 771 | 965 | 345 | 576 | 924 |
| 077 | 423 | 465 | 993 | 661 | -243 | -937 | -820 | 006 | 827 | 932 | 230 | 577 | 923 |
| 078 | 422 | 471 | 995 | 637 | -285 | -955 | -778 | 088 | 876 | 888 | 113 | 578 | 922 |
| 079 | 421 | 476 | 997 | 613 | -327 | -970 | -733 | 169 | 918 | 834 | -006 | 579 | 921 |
| 080 | 420 | 482 | 998 | 588 | -368 | -982 | -685 | 249 | 951 | 771 | -125 | 580 | 920 |
| 081 | 419 | 487 | 999 | 562 | -409 | -991 | -633 | 327 | 976 | 698 | -243 | 581 | 919 |
| 082 | 418 | 493 | 1000 | 536 | -448 | -997 | -578 | 403 | 992 | 618 | -356 | 582 | 918 |
| 083 | 417 | 498 | 1000 | 509 | -487 | -1000 | -520 | 476 | 1000 | 531 | -465 | 583 | 917 |
| 084 | 416 | 504 | 1000 | 482 | -525 | -999 | -460 | 546 | 998 | 437 | -567 | 584 | 916 |

TABLE 8.5A (continued)

 $\sin 2\pi hx$ (h odd) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=21$ | 23 | 25 | 27 | 29 | 31 | 33 | 35 | 37 | 39 | Change sign.
x | |
|-----------------------|-----|--------|-------|-------|-------|------|------|-------|-------|------|-------|---------------------|-----|
| 040 | 460 | −844 | −482 | 000 | 482 | 844 | 998 | 905 | 588 | 125 | −368 | 540 | 960 |
| 041 | 459 | −767 | −351 | 156 | 623 | 927 | 991 | 798 | 397 | −107 | −583 | 541 | 959 |
| 042 | 458 | −675 | −212 | 309 | 746 | 980 | 947 | 657 | 187 | −333 | −762 | 542 | 958 |
| 043 | 457 | −572 | −069 | 454 | 848 | 1000 | 867 | 487 | −031 | −541 | −897 | 543 | 957 |
| 044 | 456 | −460 | 075 | 588 | 925 | 987 | 754 | 297 | −249 | −720 | −977 | 544 | 956 |
| | | | | | | | | | | | | | |
| 045 | 455 | −339 | 218 | 707 | 976 | 941 | 613 | 094 | −454 | −861 | −1000 | 545 | 955 |
| 046 | 454 | −212 | 356 | 809 | 999 | 864 | 448 | −113 | −637 | −955 | −962 | 546 | 954 |
| 047 | 453 | −082 | 487 | 891 | 993 | 758 | 267 | −315 | −790 | −998 | −867 | 547 | 953 |
| 048 | 452 | 050 | 608 | 951 | 959 | 628 | 075 | −504 | −905 | −987 | −720 | 548 | 952 |
| 049 | 451 | 181 | 716 | 988 | 897 | 476 | −119 | −671 | −976 | −923 | −531 | 549 | 951 |
| | | | | | | | | | | | | | |
| 050 | 450 | 309 | 809 | 1000 | 809 | 309 | −309 | −809 | −1000 | −809 | −309 | 550 | 950 |
| 051 | 449 | 431 | 885 | 988 | 698 | 132 | −487 | −913 | −976 | −652 | −069 | 551 | 949 |
| 052 | 448 | 546 | 943 | 951 | 567 | −050 | −647 | −977 | −905 | −460 | 175 | 552 | 948 |
| 053 | 447 | 652 | 981 | 891 | 420 | −230 | −782 | −1000 | −790 | −243 | 409 | 553 | 947 |
| 054 | 446 | 746 | 999 | 809 | 261 | −403 | −888 | −980 | −637 | −013 | 618 | 554 | 946 |
| | | | | | | | | | | | | | |
| 055 | 445 | 827 | 996 | 707 | 094 | −562 | −960 | −918 | −454 | 218 | 790 | 555 | 945 |
| 056 | 444 | 894 | 972 | 588 | −075 | −703 | −996 | −816 | −249 | 437 | 915 | 556 | 944 |
| 057 | 443 | 945 | 927 | 454 | −243 | −820 | −994 | −680 | −031 | 633 | 986 | 557 | 943 |
| 058 | 442 | 980 | 864 | 309 | −403 | −910 | −955 | −514 | 187 | 794 | 997 | 558 | 942 |
| 059 | 441 | 998 | 782 | 156 | −552 | −970 | −879 | −327 | 397 | 913 | 949 | 559 | 941 |
| | | | | | | | | | | | | | |
| 060 | 440 | 998 | 685 | 000 | −685 | −998 | −771 | −125 | 588 | 982 | 844 | 560 | 940 |
| 061 | 439 | 981 | 572 | −156 | −798 | −993 | −633 | 082 | 750 | 999 | 689 | 561 | 939 |
| 062 | 438 | 947 | 448 | −309 | −888 | −955 | −471 | 285 | 876 | 962 | 493 | 562 | 938 |
| 063 | 437 | 897 | 315 | −454 | −953 | −885 | −291 | 476 | 960 | 873 | 267 | 563 | 937 |
| 064 | 436 | 831 | 175 | −588 | −990 | −786 | −100 | 647 | 998 | 738 | 025 | 564 | 936 |
| | | | | | | | | | | | | | |
| 065 | 435 | 750 | 031 | −707 | −1000 | −661 | 094 | 790 | 988 | 562 | −218 | 565 | 935 |
| 066 | 434 | 657 | −113 | −809 | −980 | −514 | 285 | 899 | 930 | 356 | −448 | 566 | 934 |
| 067 | 433 | 552 | −255 | −891 | −932 | −351 | 465 | 970 | 827 | 132 | −652 | 567 | 933 |
| 068 | 432 | 437 | −391 | −951 | −858 | −175 | 628 | 999 | 685 | −100 | −816 | 568 | 932 |
| 069 | 431 | 315 | −520 | −988 | −758 | 006 | 767 | 986 | 509 | −327 | −932 | 569 | 931 |
| | | | | | | | | | | | | | |
| 070 | 430 | 187 | −637 | −1000 | −637 | 187 | 876 | 930 | 309 | −536 | −992 | 570 | 930 |
| 071 | 429 | 057 | −742 | −988 | −498 | 362 | 953 | 834 | 094 | −716 | −993 | 571 | 929 |
| 072 | 428 | −075 | −831 | −951 | −345 | 525 | 994 | 703 | −125 | −858 | −934 | 572 | 928 |
| 073 | 427 | −206 | −902 | −891 | −181 | 671 | 997 | 541 | −339 | −953 | −820 | 573 | 927 |
| 074 | 426 | −333 | −955 | −809 | −013 | 794 | 962 | 356 | −536 | −997 | −657 | 574 | 926 |
| | | | | | | | | | | | | | |
| 075 | 425 | −454 | −988 | −707 | 156 | 891 | 891 | 156 | −707 | −988 | −454 | 575 | 925 |
| 076 | 424 | −567 | −1000 | −588 | 321 | 959 | 786 | −050 | −844 | −925 | −224 | 576 | 924 |
| 077 | 423 | −671 | −991 | −454 | 476 | 994 | 652 | −255 | −941 | −813 | 019 | 577 | 923 |
| 078 | 422 | −762 | −962 | −309 | 618 | 997 | 493 | −448 | −992 | −657 | 261 | 578 | 922 |
| 079 | 421 | −841 | −913 | −156 | 742 | 967 | 315 | −623 | −996 | −465 | 487 | 579 | 921 |
| | | | | | | | | | | | | | |
| 080 | 420 | −905 | −844 | 000 | 844 | 905 | 125 | −771 | −951 | −249 | 685 | 580 | 920 |
| 081 | 419 | −953 | −758 | 156 | 923 | 813 | −069 | −885 | −861 | −019 | 841 | 581 | 919 |
| 082 | 418 | −985 | −657 | 309 | 975 | 694 | −261 | −962 | −729 | 212 | 947 | 582 | 918 |
| 083 | 417 | −999 | −541 | 454 | 998 | 552 | −443 | −998 | −562 | 431 | 997 | 583 | 917 |
| 084 | 416 | −996 | −414 | 588 | 994 | 391 | −608 | −990 | −368 | 628 | 987 | 584 | 916 |

TABLE 8.5A (continued)

 $\sin 2\pi hx$ (h odd) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=1$ | 3 | 5 | 7 | 9 | 11 | 13 | 15 | 17 | 19 | Change sign.
x | |
|-----------------------|-----|-------|------|------|-------|------|------|------|-------|-------|-------|---------------------|-----|
| 085 | 415 | 509 | 1000 | 454 | -562 | -996 | -397 | 613 | 988 | 339 | -661 | 585 | 915 |
| 086 | 414 | 514 | 999 | 426 | -598 | -989 | -333 | 675 | 969 | 237 | -746 | 586 | 914 |
| 087 | 413 | 520 | 998 | 397 | -633 | -979 | -267 | 733 | 941 | 132 | -820 | 587 | 913 |
| 088 | 412 | 525 | 996 | 368 | -666 | -965 | -200 | 786 | 905 | 025 | -882 | 588 | 912 |
| 089 | 411 | 531 | 994 | 339 | -698 | -949 | -132 | 834 | 861 | -082 | -932 | 589 | 911 |
| 090 | 410 | 536 | 992 | 309 | -729 | -930 | -063 | 876 | 809 | -187 | -969 | 590 | 910 |
| 091 | 409 | 541 | 990 | 279 | -758 | -907 | 006 | 913 | 750 | -291 | -991 | 591 | 909 |
| 092 | 408 | 546 | 987 | 249 | -786 | -882 | 075 | 943 | 685 | -391 | -1000 | 592 | 908 |
| 093 | 407 | 552 | 983 | 218 | -813 | -854 | 144 | 967 | 613 | -487 | -994 | 593 | 907 |
| 094 | 406 | 557 | 980 | 187 | -838 | -824 | 212 | 985 | 536 | -578 | -975 | 594 | 906 |
| 095 | 405 | 562 | 976 | 156 | -861 | -790 | 279 | 996 | 454 | -661 | -941 | 595 | 905 |
| 096 | 404 | 567 | 972 | 125 | -882 | -754 | 345 | 1000 | 368 | -738 | -894 | 596 | 904 |
| 097 | 403 | 572 | 967 | 094 | -902 | -716 | 409 | 998 | 279 | -805 | -834 | 597 | 903 |
| 098 | 402 | 578 | 962 | 063 | -920 | -675 | 471 | 989 | 187 | -864 | -762 | 598 | 902 |
| 099 | 401 | 583 | 957 | 031 | -937 | -633 | 531 | 973 | 094 | -913 | -680 | 599 | 901 |
| 100 | 400 | 588 | 951 | 000 | -951 | -588 | 588 | 951 | 000 | -951 | -588 | 600 | 900 |
| 101 | 399 | 593 | 945 | -031 | -964 | -541 | 642 | 923 | -094 | -979 | -487 | 601 | 899 |
| 102 | 398 | 598 | 939 | -063 | -975 | -493 | 694 | 888 | -187 | -995 | -380 | 602 | 898 |
| 103 | 397 | 603 | 932 | -094 | -983 | -443 | 742 | 848 | -279 | -1000 | -267 | 603 | 897 |
| 104 | 396 | 608 | 925 | -125 | -990 | -391 | 786 | 802 | -368 | -994 | -150 | 604 | 896 |
| 105 | 395 | 613 | 918 | -156 | -996 | -339 | 827 | 750 | -454 | -976 | -031 | 605 | 895 |
| 106 | 394 | 618 | 910 | -187 | -999 | -285 | 864 | 694 | -536 | -947 | 088 | 606 | 894 |
| 107 | 393 | 623 | 902 | -218 | -1000 | -230 | 897 | 633 | -613 | -907 | 206 | 607 | 893 |
| 108 | 392 | 628 | 894 | -249 | -999 | -175 | 925 | 567 | -685 | -858 | 321 | 608 | 892 |
| 109 | 391 | 633 | 885 | -279 | -997 | -119 | 949 | 498 | -750 | -798 | 431 | 609 | 891 |
| 110 | 390 | 637 | 876 | -309 | -992 | -063 | 969 | 426 | -809 | -729 | 536 | 610 | 890 |
| 111 | 389 | 642 | 867 | -339 | -986 | -006 | 983 | 351 | -861 | -652 | 633 | 611 | 889 |
| 112 | 388 | 647 | 858 | -368 | -977 | 050 | 994 | 273 | -905 | -567 | 720 | 612 | 888 |
| 113 | 387 | 652 | 848 | -397 | -967 | 107 | 999 | 194 | -941 | -476 | 798 | 613 | 887 |
| 114 | 386 | 657 | 838 | -426 | -955 | 163 | 1000 | 113 | -969 | -380 | 864 | 614 | 886 |
| 115 | 385 | 661 | 827 | -454 | -941 | 218 | 996 | 031 | -988 | -279 | 918 | 615 | 885 |
| 116 | 384 | 666 | 816 | -482 | -925 | 273 | 987 | -050 | -998 | -175 | 959 | 616 | 884 |
| 117 | 383 | 671 | 805 | -509 | -907 | 327 | 973 | -132 | -1000 | -069 | 986 | 617 | 883 |
| 118 | 382 | 675 | 794 | -536 | -888 | 380 | 955 | -212 | -992 | 038 | 999 | 618 | 882 |
| 119 | 381 | 680 | 782 | -562 | -867 | 431 | 932 | -291 | -976 | 144 | 998 | 619 | 881 |
| 120 | 380 | 685 | 771 | -588 | -844 | 482 | 905 | -368 | -951 | 249 | 982 | 620 | 880 |
| 121 | 379 | 689 | 758 | -613 | -820 | 531 | 873 | -443 | -918 | 351 | 953 | 621 | 879 |
| 122 | 378 | 694 | 746 | -637 | -794 | 578 | 838 | -514 | -876 | 448 | 910 | 622 | 878 |
| 123 | 377 | 698 | 733 | -661 | -767 | 623 | 798 | -583 | -827 | 541 | 854 | 623 | 877 |
| 124 | 376 | 703 | 720 | -685 | -738 | 666 | 754 | -647 | -771 | 628 | 786 | 624 | 876 |
| 125 | 375 | 707 | 707 | -707 | -707 | 707 | 707 | -707 | -707 | 707 | 707 | 625 | 875 |
| 126 | 374 | 712 | 694 | -729 | -675 | 746 | 657 | -762 | -637 | 778 | 618 | 626 | 874 |
| 127 | 373 | 716 | 680 | -750 | -642 | 782 | 603 | -813 | -562 | 841 | 520 | 627 | 873 |
| 128 | 372 | 720 | 666 | -771 | -608 | 816 | 546 | -858 | -482 | 894 | 414 | 628 | 872 |
| 129 | 371 | 725 | 652 | -790 | -572 | 848 | 487 | -897 | -397 | 937 | 303 | 629 | 871 |

TABLE 8.5A (continued)

 $\sin 2\pi hx$ (h odd) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=21$ | 23 | 25 | 27 | 29 | 31 | 33 | 35 | 37 | 39 | Change sign.
x | |
|-----------------------|-----|--------|------|-------|-------|-------|-------|------|-------|------|------|---------------------|-----|
| 085 | 415 | -976 | -279 | 707 | 960 | 218 | -750 | -941 | -156 | 790 | 918 | 585 | 915 |
| 086 | 414 | -939 | -138 | 809 | 899 | 038 | -864 | -851 | 063 | 910 | 794 | 586 | 914 |
| 087 | 413 | -885 | 006 | 891 | 813 | -144 | -945 | -725 | 279 | 981 | 623 | 587 | 913 |
| 088 | 412 | -816 | 150 | 951 | 703 | -321 | -990 | -567 | 482 | 999 | 414 | 588 | 912 |
| 089 | 411 | -733 | 291 | 988 | 572 | -487 | -998 | -386 | 661 | 964 | 181 | 589 | 911 |
| | | | | | | | | | | | | | |
| 090 | 410 | -637 | 426 | 1000 | 426 | -637 | -969 | -187 | 809 | 876 | -063 | 590 | 910 |
| 091 | 409 | -531 | 552 | 988 | 267 | -767 | -902 | 019 | 918 | 742 | -303 | 591 | 909 |
| 092 | 408 | -414 | 666 | 951 | 100 | -870 | -802 | 224 | 982 | 567 | -525 | 592 | 908 |
| 093 | 407 | -291 | 767 | 891 | -069 | -945 | -671 | 420 | 1000 | 362 | -716 | 593 | 907 |
| 094 | 406 | -163 | 851 | 809 | -237 | -989 | -514 | 598 | 969 | 138 | -864 | 594 | 906 |
| | | | | | | | | | | | | | |
| 095 | 405 | -031 | 918 | 707 | -397 | -1000 | -339 | 750 | 891 | -094 | -960 | 595 | 905 |
| 096 | 404 | 100 | 965 | 588 | -546 | -977 | -150 | 870 | 771 | -321 | -999 | 596 | 904 |
| 097 | 403 | 230 | 993 | 454 | -680 | -923 | 044 | 953 | 613 | -531 | -979 | 597 | 903 |
| 098 | 402 | 356 | 1000 | 309 | -794 | -838 | 237 | 995 | 426 | -712 | -899 | 598 | 902 |
| 099 | 401 | 476 | 986 | 156 | -885 | -725 | 420 | 994 | 218 | -854 | -767 | 599 | 901 |
| | | | | | | | | | | | | | |
| 100 | 400 | 588 | 951 | 000 | -951 | -588 | 588 | 951 | 000 | -951 | -588 | 600 | 900 |
| 101 | 399 | 689 | 897 | -156 | -990 | -431 | 733 | 867 | -218 | -997 | -374 | 601 | 899 |
| 102 | 398 | 778 | 824 | -309 | -1000 | -261 | 851 | 746 | -426 | -989 | -138 | 602 | 898 |
| 103 | 397 | 854 | 733 | -454 | -981 | -082 | 937 | 593 | -613 | -927 | 107 | 603 | 897 |
| 104 | 396 | 915 | 628 | -588 | -934 | 100 | 987 | 414 | -771 | -816 | 345 | 604 | 896 |
| | | | | | | | | | | | | | |
| 105 | 395 | 960 | 509 | -707 | -861 | 279 | 1000 | 218 | -891 | -661 | 562 | 605 | 895 |
| 106 | 394 | 989 | 380 | -809 | -762 | 448 | 975 | 013 | -969 | -471 | 746 | 606 | 894 |
| 107 | 393 | 1000 | 243 | -891 | -642 | 603 | 913 | -194 | -1000 | -255 | 885 | 607 | 893 |
| 108 | 392 | 994 | 100 | -951 | -504 | 738 | 816 | -391 | -982 | -025 | 972 | 608 | 892 |
| 109 | 391 | 970 | -044 | -988 | -351 | 848 | 689 | -572 | -918 | 206 | 1000 | 609 | 891 |
| | | | | | | | | | | | | | |
| 110 | 390 | 930 | -187 | -1000 | -187 | 930 | 536 | -729 | -809 | 426 | 969 | 610 | 890 |
| 111 | 389 | 873 | -327 | -988 | -019 | 981 | 362 | -854 | -661 | 623 | 879 | 611 | 889 |
| 112 | 388 | 802 | -460 | -951 | 150 | 1000 | 175 | -943 | -482 | 786 | 738 | 612 | 888 |
| 113 | 387 | 716 | -583 | -891 | 315 | 986 | -019 | -991 | -279 | 907 | 552 | 613 | 887 |
| 114 | 386 | 618 | -694 | -809 | 471 | 939 | -212 | -997 | -063 | 980 | 333 | 614 | 886 |
| | | | | | | | | | | | | | |
| 115 | 385 | 509 | -790 | -707 | 613 | 861 | -397 | -960 | 156 | 1000 | 094 | 615 | 885 |
| 116 | 384 | 391 | -870 | -588 | 738 | 754 | -567 | -882 | 368 | 965 | -150 | 616 | 884 |
| 117 | 383 | 267 | -932 | -454 | 841 | 623 | -716 | -767 | 562 | 879 | -386 | 617 | 883 |
| 118 | 382 | 138 | -975 | -309 | 920 | 471 | -838 | -618 | 729 | 746 | -598 | 618 | 882 |
| 119 | 381 | 006 | -997 | -156 | 973 | 303 | -927 | -443 | 861 | 572 | -775 | 619 | 881 |
| | | | | | | | | | | | | | |
| 120 | 380 | -125 | -998 | 000 | 998 | 125 | -982 | -249 | 951 | 368 | -905 | 620 | 880 |
| 121 | 379 | -255 | -979 | 156 | 994 | -057 | -1000 | -044 | 996 | 144 | -981 | 621 | 879 |
| 122 | 378 | -380 | -939 | 309 | 962 | -237 | -980 | 163 | 992 | -088 | -999 | 622 | 878 |
| 123 | 377 | -498 | -879 | 454 | 902 | -409 | -923 | 362 | 941 | -315 | -957 | 623 | 877 |
| 124 | 376 | -608 | -802 | 588 | 816 | -567 | -831 | 546 | 844 | -525 | -858 | 624 | 876 |
| | | | | | | | | | | | | | |
| 125 | 375 | -707 | -707 | 707 | 707 | -707 | -707 | 707 | 707 | -707 | -707 | 625 | 875 |
| 126 | 374 | -794 | -598 | 809 | 578 | -824 | -557 | 838 | 536 | -851 | -514 | 626 | 874 |
| 127 | 373 | -867 | -476 | 891 | 431 | -913 | -386 | 932 | 339 | -949 | -291 | 627 | 873 |
| 128 | 372 | -925 | -345 | 951 | 273 | -972 | -200 | 987 | 125 | -996 | -050 | 628 | 872 |
| 129 | 371 | -967 | -206 | 988 | 107 | -998 | -006 | 999 | -094 | -990 | 194 | 629 | 871 |

TABLE 8.5A (*continued*)
 $\sin 2\pi hx$ (h odd) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=1$ | 3 | 5 | 7 | 9 | 11 | 13 | 15 | 17 | 19 | Change sign.
x | |
|-----------------------|-----|-------|------|-------|------|------|-------|-------|------|-------|-------|---------------------|-----|
| 130 | 370 | 729 | 637 | -809 | -536 | 876 | 426 | -930 | -309 | 969 | 187 | 630 | 870 |
| 131 | 369 | 733 | 623 | -827 | -498 | 902 | 362 | -957 | -218 | 990 | 069 | 631 | 869 |
| 132 | 368 | 738 | 608 | -844 | -460 | 925 | 297 | -977 | -125 | 999 | -050 | 632 | 868 |
| 133 | 367 | 742 | 593 | -861 | -420 | 945 | 230 | -991 | -031 | 998 | -169 | 633 | 867 |
| 134 | 366 | 746 | 578 | -876 | -380 | 962 | 163 | -999 | 063 | 985 | -285 | 634 | 866 |
| | | | | | | | | | | | | | |
| 135 | 365 | 750 | 562 | -891 | -339 | 976 | 094 | -1000 | 156 | 960 | -397 | 635 | 865 |
| 136 | 364 | 754 | 546 | -905 | -297 | 987 | 025 | -994 | 249 | 925 | -504 | 636 | 864 |
| 137 | 363 | 758 | 531 | -918 | -255 | 994 | -044 | -981 | 339 | 879 | -603 | 637 | 863 |
| 138 | 362 | 762 | 514 | -930 | -212 | 999 | -113 | -962 | 426 | 824 | -694 | 638 | 862 |
| 139 | 361 | 767 | 498 | -941 | -169 | 1000 | -181 | -937 | 509 | 758 | -775 | 639 | 861 |
| | | | | | | | | | | | | | |
| 140 | 360 | 771 | 482 | -951 | -125 | 998 | -249 | -905 | 588 | 685 | -844 | 640 | 860 |
| 141 | 359 | 775 | 465 | -960 | -082 | 993 | -315 | -867 | 661 | 603 | -902 | 641 | 859 |
| 142 | 358 | 778 | 448 | -969 | -038 | 985 | -380 | -824 | 729 | 514 | -947 | 642 | 858 |
| 143 | 357 | 782 | 431 | -976 | 006 | 973 | -443 | -775 | 790 | 420 | -979 | 643 | 857 |
| 144 | 356 | 786 | 414 | -982 | 050 | 959 | -504 | -720 | 844 | 321 | -996 | 644 | 856 |
| | | | | | | | | | | | | | |
| 145 | 355 | 790 | 397 | -988 | 094 | 941 | -562 | -661 | 891 | 218 | -1000 | 645 | 855 |
| 146 | 354 | 794 | 380 | -992 | 138 | 920 | -618 | -598 | 930 | 113 | -989 | 646 | 854 |
| 147 | 353 | 798 | 362 | -996 | 181 | 897 | -671 | -531 | 960 | 006 | -964 | 647 | 853 |
| 148 | 352 | 802 | 345 | -998 | 224 | 870 | -720 | -460 | 982 | -100 | -925 | 648 | 852 |
| 149 | 351 | 805 | 327 | -1000 | 267 | 841 | -767 | -386 | 996 | -206 | -873 | 649 | 851 |
| | | | | | | | | | | | | | |
| 150 | 350 | 809 | 309 | -1000 | 309 | 809 | -809 | -309 | 1000 | -309 | -809 | 650 | 850 |
| 151 | 349 | 813 | 291 | -1000 | 351 | 775 | -848 | -230 | 996 | -409 | -733 | 651 | 849 |
| 152 | 348 | 816 | 273 | -998 | 391 | 738 | -882 | -150 | 982 | -504 | -647 | 652 | 848 |
| 153 | 347 | 820 | 255 | -996 | 431 | 698 | -913 | -069 | 960 | -593 | -552 | 653 | 847 |
| 154 | 346 | 824 | 237 | -992 | 471 | 657 | -939 | 013 | 930 | -675 | -448 | 654 | 846 |
| | | | | | | | | | | | | | |
| 155 | 345 | 827 | 218 | -988 | 509 | 613 | -960 | 094 | 891 | -750 | -339 | 655 | 845 |
| 156 | 344 | 831 | 200 | -982 | 546 | 567 | -977 | 175 | 844 | -816 | -224 | 656 | 844 |
| 157 | 343 | 834 | 181 | -976 | 583 | 520 | -990 | 255 | 790 | -873 | -107 | 657 | 843 |
| 158 | 342 | 838 | 163 | -969 | 618 | 471 | -997 | 333 | 729 | -920 | 013 | 658 | 842 |
| 159 | 341 | 841 | 144 | -960 | 652 | 420 | -1000 | 409 | 661 | -957 | 132 | 659 | 841 |
| | | | | | | | | | | | | | |
| 160 | 340 | 844 | 125 | -951 | 685 | 368 | -998 | 482 | 588 | -982 | 249 | 660 | 840 |
| 161 | 339 | 848 | 107 | -941 | 716 | 315 | -991 | 552 | 509 | -997 | 362 | 661 | 839 |
| 162 | 338 | 851 | 088 | -930 | 746 | 261 | -980 | 618 | 426 | -1000 | 471 | 662 | 838 |
| 163 | 337 | 854 | 069 | -918 | 775 | 206 | -964 | 680 | 339 | -991 | 572 | 663 | 837 |
| 164 | 336 | 858 | 050 | -905 | 802 | 150 | -943 | 738 | 249 | -972 | 666 | 664 | 836 |
| | | | | | | | | | | | | | |
| 165 | 335 | 861 | 031 | -891 | 827 | 094 | -918 | 790 | 156 | -941 | 750 | 665 | 835 |
| 166 | 334 | 864 | 013 | -876 | 851 | 038 | -888 | 838 | 063 | -899 | 824 | 666 | 834 |
| 167 | 333 | 867 | -006 | -861 | 873 | -019 | -854 | 879 | -031 | -848 | 885 | 667 | 833 |
| 168 | 332 | 870 | -025 | -844 | 894 | -075 | -816 | 915 | -125 | -786 | 934 | 668 | 832 |
| 169 | 331 | 873 | -044 | -827 | 913 | -132 | -775 | 945 | -218 | -716 | 970 | 669 | 831 |
| | | | | | | | | | | | | | |
| 170 | 330 | 876 | -063 | -809 | 930 | -187 | -729 | 969 | -309 | -637 | 992 | 670 | 830 |
| 171 | 329 | 879 | -082 | -790 | 945 | -243 | -680 | 986 | -397 | -552 | 1000 | 671 | 829 |
| 172 | 328 | 882 | -100 | -771 | 959 | -297 | -628 | 996 | -482 | -460 | 994 | 672 | 828 |
| 173 | 327 | 885 | -119 | -750 | 970 | -351 | -572 | 1000 | -562 | -362 | 973 | 673 | 827 |
| 174 | 326 | 888 | -138 | -729 | 980 | -403 | -514 | 997 | -637 | -261 | 939 | 674 | 826 |

TABLE 8.5A (continued)

 $\sin 2\pi hx$ (h odd) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=21$ | 23 | 25 | 27 | 29 | 31 | 33 | 35 | 37 | 39 | Change sign.
x | |
|-----------------------|-----|--------|-------|-------|-------|------|------|-------|------|------|-------|---------------------|-----|
| 130 | 370 | −992 | −063 | 1000 | −063 | −992 | 187 | 969 | −309 | −930 | 426 | 630 | 870 |
| 131 | 369 | −1000 | 082 | 988 | −230 | −953 | 374 | 897 | −509 | −820 | 633 | 631 | 869 |
| 132 | 368 | −990 | 224 | 951 | −391 | −882 | 546 | 786 | −685 | −666 | 802 | 632 | 868 |
| 133 | 367 | −964 | 362 | 891 | −541 | −782 | 698 | 642 | −827 | −476 | 923 | 633 | 867 |
| 134 | 366 | −920 | 493 | 809 | −675 | −657 | 824 | 471 | −930 | −261 | 989 | 634 | 866 |
| | | | | | | | | | | | | | |
| 135 | 365 | −861 | 613 | 707 | −790 | −509 | 918 | 279 | −988 | −031 | 996 | 635 | 865 |
| 136 | 364 | −786 | 720 | 588 | −882 | −345 | 977 | 075 | −998 | 200 | 943 | 636 | 864 |
| 137 | 363 | −698 | 813 | 454 | −949 | −169 | 1000 | −132 | −960 | 420 | 834 | 637 | 863 |
| 138 | 362 | −598 | 888 | 309 | −989 | 013 | 985 | −333 | −876 | 618 | 675 | 638 | 862 |
| 139 | 361 | −487 | 945 | 156 | −1000 | 194 | 932 | −520 | −750 | 782 | 476 | 639 | 861 |
| | | | | | | | | | | | | | |
| 140 | 360 | −368 | 982 | 000 | −982 | 368 | 844 | −685 | −588 | 905 | 249 | 640 | 860 |
| 141 | 359 | −243 | 999 | −156 | −937 | 531 | 725 | −820 | −397 | 979 | 006 | 641 | 859 |
| 142 | 358 | −113 | 995 | −309 | −864 | 675 | 578 | −920 | −187 | 1000 | −237 | 642 | 858 |
| 143 | 357 | 019 | 970 | −454 | −767 | 798 | 409 | −981 | 031 | 967 | −465 | 643 | 857 |
| 144 | 356 | 150 | 925 | −588 | −647 | 894 | 224 | −1000 | 249 | 882 | −666 | 644 | 856 |
| | | | | | | | | | | | | | |
| 145 | 355 | 279 | 861 | −707 | −509 | 960 | 031 | −976 | 454 | 750 | −827 | 645 | 855 |
| 146 | 354 | 403 | 778 | −809 | −356 | 995 | −163 | −910 | 637 | 578 | −939 | 646 | 854 |
| 147 | 353 | 520 | 680 | −891 | −194 | 997 | −351 | −805 | 790 | 374 | −994 | 647 | 853 |
| 148 | 352 | 628 | 567 | −951 | −025 | 965 | −525 | −666 | 905 | 150 | −990 | 648 | 852 |
| 149 | 351 | 725 | 443 | −988 | 144 | 902 | −680 | −498 | 976 | −082 | −927 | 649 | 851 |
| | | | | | | | | | | | | | |
| 150 | 350 | 809 | 309 | −1000 | 309 | 809 | −809 | −309 | 1000 | −309 | −809 | 650 | 850 |
| 151 | 349 | 879 | 169 | −988 | 465 | 689 | −907 | −107 | 976 | −520 | −642 | 651 | 849 |
| 152 | 348 | 934 | 025 | −951 | 608 | 546 | −972 | 100 | 905 | −703 | −437 | 652 | 848 |
| 153 | 347 | 973 | −119 | −891 | 733 | 386 | −999 | 303 | 790 | −848 | −206 | 653 | 847 |
| 154 | 346 | 995 | −261 | −809 | 838 | 212 | −989 | 493 | 637 | −947 | 038 | 654 | 846 |
| | | | | | | | | | | | | | |
| 155 | 345 | 1000 | −397 | −707 | 918 | 031 | −941 | 661 | 454 | −996 | 279 | 655 | 845 |
| 156 | 344 | 987 | −525 | −588 | 972 | −150 | −858 | 802 | 249 | −990 | 504 | 656 | 844 |
| 157 | 343 | 957 | −642 | −454 | 998 | −327 | −742 | 907 | 031 | −932 | 698 | 657 | 843 |
| 158 | 342 | 910 | −746 | −309 | 995 | −493 | −598 | 975 | −187 | −824 | 851 | 658 | 842 |
| 159 | 341 | 848 | −834 | −156 | 964 | −642 | −431 | 1000 | −397 | −671 | 953 | 659 | 841 |
| | | | | | | | | | | | | | |
| 160 | 340 | 771 | −905 | 000 | 905 | −771 | −249 | 982 | −588 | −482 | 998 | 660 | 840 |
| 161 | 339 | 680 | −957 | 156 | 820 | −873 | −057 | 923 | −750 | −267 | 983 | 661 | 839 |
| 162 | 338 | 578 | −989 | 309 | 712 | −947 | 138 | 824 | −876 | −038 | 910 | 662 | 838 |
| 163 | 337 | 465 | −1000 | 454 | 583 | −990 | 327 | 689 | −960 | 194 | 782 | 663 | 837 |
| 164 | 336 | 345 | −990 | 588 | 437 | −999 | 504 | 525 | −998 | 414 | 608 | 664 | 836 |
| | | | | | | | | | | | | | |
| 165 | 335 | 218 | −960 | 707 | 279 | −976 | 661 | 339 | −988 | 613 | 397 | 665 | 835 |
| 166 | 334 | 088 | −910 | 809 | 113 | −920 | 794 | 138 | −930 | 778 | 163 | 666 | 834 |
| 167 | 333 | −044 | −841 | 891 | −057 | −834 | 897 | −069 | −827 | 902 | −082 | 667 | 833 |
| 168 | 332 | −175 | −754 | 951 | −224 | −720 | 965 | −273 | −685 | 977 | −321 | 668 | 832 |
| 169 | 331 | −303 | −652 | 988 | −386 | −583 | 998 | −465 | −509 | 1000 | −541 | 669 | 831 |
| | | | | | | | | | | | | | |
| 170 | 330 | −426 | −536 | 1000 | −536 | −426 | 992 | −637 | −309 | 969 | −729 | 670 | 830 |
| 171 | 329 | −541 | −409 | 988 | −671 | −255 | 949 | −782 | −094 | 885 | −873 | 671 | 829 |
| 172 | 328 | −647 | −273 | 951 | −786 | −075 | 870 | −894 | 125 | 754 | −965 | 672 | 828 |
| 173 | 327 | −742 | −132 | 891 | −879 | 107 | 758 | −967 | 339 | 583 | −1000 | 673 | 827 |
| 174 | 326 | −824 | 013 | 809 | −947 | 285 | 618 | −999 | 536 | 380 | −975 | 674 | 826 |

TABLE 8.5A (*continued*)
 $\sin 2\pi hx$ (h odd) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=1$ | 3 | 5 | 7 | 9 | 11 | 13 | 15 | 17 | 19 | Change sign.
x | |
|-----------------------|-----|-------|------|------|------|-------|------|------|-------|------|------|---------------------|-----|
| 175 | 325 | 891 | -156 | -707 | 988 | -454 | -454 | 988 | -707 | -156 | 891 | 675 | 825 |
| 176 | 324 | 894 | -175 | -685 | 994 | -504 | -391 | 972 | -771 | -050 | 831 | 676 | 824 |
| 177 | 323 | 897 | -194 | -661 | 998 | -552 | -327 | 949 | -827 | 057 | 758 | 677 | 823 |
| 178 | 322 | 899 | -212 | -637 | 1000 | -598 | -261 | 920 | -876 | 163 | 675 | 678 | 822 |
| 179 | 321 | 902 | -230 | -613 | 1000 | -642 | -194 | 885 | -918 | 267 | 583 | 679 | 821 |
| | | | | | | | | | | | | | |
| 180 | 320 | 905 | -249 | -588 | 998 | -685 | -125 | 844 | -951 | 368 | 482 | 680 | 820 |
| 181 | 319 | 907 | -267 | -562 | 994 | -725 | -057 | 798 | -976 | 465 | 374 | 681 | 819 |
| 182 | 318 | 910 | -285 | -536 | 989 | -762 | 013 | 746 | -992 | 557 | 261 | 682 | 818 |
| 183 | 317 | 913 | -303 | -509 | 981 | -798 | 082 | 689 | -1000 | 642 | 144 | 683 | 817 |
| 184 | 316 | 915 | -321 | -482 | 972 | -831 | 150 | 628 | -998 | 720 | 025 | 684 | 816 |
| | | | | | | | | | | | | | |
| 185 | 315 | 918 | -339 | -454 | 960 | -861 | 218 | 562 | -988 | 790 | -094 | 685 | 815 |
| 186 | 314 | 920 | -356 | -426 | 947 | -888 | 285 | 493 | -969 | 851 | -212 | 686 | 814 |
| 187 | 313 | 923 | -374 | -397 | 932 | -913 | 351 | 420 | -941 | 902 | -327 | 687 | 813 |
| 188 | 312 | 925 | -391 | -368 | 915 | -934 | 414 | 345 | -905 | 943 | -437 | 688 | 812 |
| 189 | 311 | 927 | -409 | -339 | 897 | -953 | 476 | 267 | -861 | 973 | -541 | 689 | 811 |
| | | | | | | | | | | | | | |
| 190 | 310 | 930 | -426 | -309 | 876 | -969 | 536 | 187 | -809 | 992 | -637 | 690 | 810 |
| 191 | 309 | 932 | -443 | -279 | 854 | -981 | 593 | 107 | -750 | 1000 | -725 | 691 | 809 |
| 192 | 308 | 934 | -460 | -249 | 831 | -990 | 647 | 025 | -685 | 996 | -802 | 692 | 808 |
| 193 | 307 | 937 | -476 | -218 | 805 | -997 | 698 | -057 | -613 | 981 | -867 | 693 | 807 |
| 194 | 306 | 939 | -493 | -187 | 778 | -1000 | 746 | -138 | -536 | 955 | -920 | 694 | 806 |
| | | | | | | | | | | | | | |
| 195 | 305 | 941 | -509 | -156 | 750 | -1000 | 790 | -218 | -454 | 918 | -960 | 695 | 805 |
| 196 | 304 | 943 | -525 | -125 | 720 | -996 | 831 | -297 | -368 | 870 | -987 | 696 | 804 |
| 197 | 303 | 945 | -541 | -094 | 689 | -990 | 867 | -374 | -279 | 813 | -999 | 697 | 803 |
| 198 | 302 | 947 | -557 | -063 | 657 | -980 | 899 | -448 | -187 | 746 | -997 | 698 | 802 |
| 199 | 301 | 949 | -572 | -031 | 623 | -967 | 927 | -520 | -094 | 671 | -981 | 699 | 801 |
| | | | | | | | | | | | | | |
| 200 | 300 | 951 | -588 | 000 | 588 | -951 | 951 | -588 | 000 | 588 | -951 | 700 | 800 |
| 201 | 299 | 953 | -603 | 031 | 552 | -932 | 970 | -652 | 094 | 498 | -907 | 701 | 799 |
| 202 | 298 | 955 | -618 | 063 | 514 | -910 | 985 | -712 | 187 | 403 | -851 | 702 | 798 |
| 203 | 297 | 957 | -633 | 094 | 476 | -885 | 994 | -767 | 279 | 303 | -782 | 703 | 797 |
| 204 | 296 | 959 | -647 | 125 | 437 | -858 | 999 | -816 | 368 | 200 | -703 | 704 | 796 |
| | | | | | | | | | | | | | |
| 205 | 295 | 960 | -661 | 156 | 397 | -827 | 1000 | -861 | 454 | 094 | -613 | 705 | 795 |
| 206 | 294 | 962 | -675 | 187 | 356 | -794 | 995 | -899 | 536 | -013 | -514 | 706 | 794 |
| 207 | 293 | 964 | -689 | 218 | 315 | -758 | 986 | -932 | 613 | -119 | -409 | 707 | 793 |
| 208 | 292 | 965 | -703 | 249 | 273 | -720 | 972 | -959 | 685 | -224 | -297 | 708 | 792 |
| 209 | 291 | 967 | -716 | 279 | 230 | -680 | 953 | -979 | 750 | -327 | -181 | 709 | 791 |
| | | | | | | | | | | | | | |
| 210 | 290 | 969 | -729 | 309 | 187 | -637 | 930 | -992 | 809 | -426 | -063 | 710 | 790 |
| 211 | 289 | 970 | -742 | 339 | 144 | -593 | 902 | -999 | 861 | -520 | 057 | 711 | 789 |
| 212 | 288 | 972 | -754 | 368 | 100 | -546 | 870 | -999 | 905 | -608 | 175 | 712 | 788 |
| 213 | 287 | 973 | -767 | 397 | 057 | -498 | 834 | -993 | 941 | -689 | 291 | 713 | 787 |
| 214 | 286 | 975 | -778 | 426 | 013 | -448 | 794 | -980 | 969 | -762 | 403 | 714 | 786 |
| | | | | | | | | | | | | | |
| 215 | 285 | 976 | -790 | 454 | -031 | -397 | 750 | -960 | 988 | -827 | 509 | 715 | 785 |
| 216 | 284 | 977 | -802 | 482 | -075 | -345 | 703 | -934 | 998 | -882 | 608 | 716 | 784 |
| 217 | 283 | 979 | -813 | 509 | -119 | -291 | 652 | -902 | 1000 | -927 | 698 | 717 | 783 |
| 218 | 282 | 980 | -824 | 536 | -163 | -237 | 598 | -864 | 992 | -962 | 778 | 718 | 782 |
| 219 | 281 | 981 | -834 | 562 | -206 | -181 | 541 | -820 | 976 | -986 | 848 | 719 | 781 |

TABLE 8.5A (continued)

 $\sin 2\pi hx$ (h odd) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=21$ | 23 | 25 | 27 | 29 | 31 | 33 | 35 | 37 | 39 | Change sign.
x | |
|-----------------------|-----|--------|------|-------|-------|------|------|------|-------|------|------|---------------------|-----|
| 175 | 325 | −891 | 156 | 707 | −988 | 454 | 454 | −988 | 707 | 156 | −891 | 675 | 825 |
| 176 | 324 | −943 | 297 | 588 | −1000 | 608 | 273 | −934 | 844 | −075 | −754 | 676 | 824 |
| 177 | 323 | −979 | 431 | 454 | −983 | 742 | 082 | −841 | 941 | −303 | −572 | 677 | 823 |
| 178 | 322 | −997 | 557 | 309 | −939 | 851 | −113 | −712 | 992 | −514 | −356 | 678 | 822 |
| 179 | 321 | −998 | 671 | 156 | −867 | 932 | −303 | −552 | 996 | −698 | −119 | 679 | 821 |
| | | | | | | | | | | | | | |
| 180 | 320 | −982 | 771 | 000 | −771 | 982 | −482 | −368 | 951 | −844 | 125 | 680 | 820 |
| 181 | 319 | −949 | 854 | −156 | −652 | 1000 | −642 | −169 | 861 | −945 | 362 | 681 | 819 |
| 182 | 318 | −899 | 920 | −309 | −514 | 985 | −778 | 038 | 729 | −995 | 578 | 682 | 818 |
| 183 | 317 | −834 | 967 | −454 | −362 | 937 | −885 | 243 | 562 | −991 | 758 | 683 | 817 |
| 184 | 316 | −754 | 994 | −588 | −200 | 858 | −959 | 437 | 368 | −934 | 894 | 684 | 816 |
| | | | | | | | | | | | | | |
| 185 | 315 | −661 | 1000 | −707 | −031 | 750 | −996 | 613 | 156 | −827 | 976 | 685 | 815 |
| 186 | 314 | −557 | 985 | −809 | 138 | 618 | −995 | 762 | −063 | −675 | 1000 | 686 | 814 |
| 187 | 313 | −443 | 949 | −891 | 303 | 465 | −957 | 879 | −279 | −487 | 964 | 687 | 813 |
| 188 | 312 | −321 | 894 | −951 | 460 | 297 | −882 | 959 | −482 | −273 | 870 | 688 | 812 |
| 189 | 311 | −194 | 820 | −988 | 603 | 119 | −775 | 997 | −661 | −044 | 725 | 689 | 811 |
| | | | | | | | | | | | | | |
| 190 | 310 | −063 | 729 | −1000 | 729 | −063 | −637 | 992 | −809 | 187 | 536 | 690 | 810 |
| 191 | 309 | 069 | 623 | −988 | 834 | −243 | −476 | 945 | −918 | 409 | 315 | 691 | 809 |
| 192 | 308 | 200 | 504 | −951 | 915 | −414 | −297 | 858 | −982 | 608 | 075 | 692 | 808 |
| 193 | 307 | 327 | 374 | −891 | 970 | −572 | −107 | 733 | −1000 | 775 | −169 | 693 | 807 |
| 194 | 306 | 448 | 237 | −809 | 997 | −712 | 088 | 578 | −969 | 899 | −403 | 694 | 806 |
| | | | | | | | | | | | | | |
| 195 | 305 | 562 | 094 | −707 | 996 | −827 | 279 | 397 | −891 | 976 | −613 | 695 | 805 |
| 196 | 304 | 666 | −050 | −588 | 965 | −915 | 460 | 200 | −771 | 1000 | −786 | 696 | 804 |
| 197 | 303 | 758 | −194 | −454 | 907 | −973 | 623 | −006 | −613 | 970 | −913 | 697 | 803 |
| 198 | 302 | 838 | −333 | −309 | 824 | −999 | 762 | −212 | −426 | 888 | −985 | 698 | 802 |
| 199 | 301 | 902 | −465 | −156 | 716 | −991 | 873 | −409 | −218 | 758 | −998 | 699 | 801 |
| | | | | | | | | | | | | | |
| 200 | 300 | 951 | −588 | 000 | 588 | −951 | 951 | −588 | 000 | 588 | −951 | 700 | 800 |
| 201 | 299 | 983 | −698 | 156 | 443 | −879 | 993 | −742 | 218 | 386 | −848 | 701 | 799 |
| 202 | 298 | 999 | −794 | 309 | 285 | −778 | 997 | −864 | 426 | 163 | −694 | 702 | 798 |
| 203 | 297 | 997 | −873 | 454 | 119 | −652 | 964 | −949 | 613 | −069 | −498 | 703 | 797 |
| 204 | 296 | 977 | −934 | 588 | −050 | −504 | 894 | −994 | 771 | −297 | −273 | 704 | 796 |
| | | | | | | | | | | | | | |
| 205 | 295 | 941 | −976 | 707 | −218 | −339 | 790 | −996 | 891 | −509 | −031 | 705 | 795 |
| 206 | 294 | 888 | −997 | 809 | −380 | −163 | 657 | −955 | 969 | −694 | 212 | 706 | 794 |
| 207 | 293 | 820 | −998 | 891 | −531 | 019 | 498 | −873 | 1000 | −841 | 443 | 707 | 793 |
| 208 | 292 | 738 | −977 | 951 | −666 | 200 | 321 | −754 | 982 | −943 | 647 | 708 | 792 |
| 209 | 291 | 642 | −937 | 988 | −782 | 374 | 132 | −603 | 918 | −994 | 813 | 709 | 791 |
| | | | | | | | | | | | | | |
| 210 | 290 | 536 | −876 | 1000 | −876 | 536 | −063 | −426 | 809 | −992 | 930 | 710 | 790 |
| 211 | 289 | 420 | −798 | 988 | −945 | 680 | −255 | −230 | 661 | −937 | 991 | 711 | 789 |
| 212 | 288 | 297 | −703 | 951 | −987 | 802 | −437 | −025 | 482 | −831 | 994 | 712 | 788 |
| 213 | 287 | 169 | −593 | 891 | −1000 | 897 | −603 | 181 | 279 | −680 | 937 | 713 | 787 |
| 214 | 286 | 038 | −471 | 809 | −985 | 962 | −746 | 380 | 063 | −493 | 824 | 714 | 786 |
| | | | | | | | | | | | | | |
| 215 | 285 | −094 | −339 | 707 | −941 | 996 | −861 | 562 | −156 | −279 | 661 | 715 | 785 |
| 216 | 284 | −224 | −200 | 588 | −870 | 996 | −943 | 720 | −368 | −050 | 460 | 716 | 784 |
| 217 | 283 | −351 | −057 | 454 | −775 | 964 | −990 | 848 | −562 | 181 | 230 | 717 | 783 |
| 218 | 282 | −471 | 088 | 309 | −657 | 899 | −999 | 939 | −729 | 403 | −013 | 718 | 782 |
| 219 | 281 | −583 | 230 | 156 | −520 | 805 | −970 | 990 | −861 | 603 | −255 | 719 | 781 |

TABLE 8.5A (*continued*)
 $\sin 2\pi hx$ (h odd) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=1$ | 3 | 5 | 7 | 9 | 11 | 13 | 15 | 17 | 19 | Change sign.
x | |
|-----------------------|-----|-------|-------|------|-------|------|-------|------|-------|------|-------|---------------------|-----|
| 220 | 280 | 982 | -844 | 588 | -249 | -125 | 482 | -771 | 951 | -998 | 905 | 720 | 780 |
| 221 | 279 | 983 | -854 | 613 | -291 | -069 | 420 | -716 | 918 | -999 | 949 | 721 | 779 |
| 222 | 278 | 985 | -864 | 637 | -333 | -013 | 356 | -657 | 876 | -989 | 980 | 722 | 778 |
| 223 | 277 | 986 | -873 | 661 | -374 | 044 | 291 | -593 | 827 | -967 | 997 | 723 | 777 |
| 224 | 276 | 987 | -882 | 685 | -414 | 100 | 224 | -525 | 771 | -934 | 999 | 724 | 776 |
| | | | | | | | | | | | | | |
| 225 | 275 | 988 | -891 | 707 | -454 | 156 | 156 | -454 | 707 | -891 | 988 | 725 | 775 |
| 226 | 274 | 989 | -899 | 729 | -493 | 212 | 088 | -380 | 637 | -838 | 962 | 726 | 774 |
| 227 | 273 | 990 | -907 | 750 | -531 | 267 | 019 | -303 | 562 | -775 | 923 | 727 | 773 |
| 228 | 272 | 990 | -915 | 771 | -567 | 321 | -050 | -224 | 482 | -703 | 870 | 728 | 772 |
| 229 | 271 | 991 | -923 | 790 | -603 | 374 | -119 | -144 | 397 | -623 | 805 | 729 | 771 |
| | | | | | | | | | | | | | |
| 230 | 270 | 992 | -930 | 809 | -637 | 426 | -187 | -063 | 309 | -536 | 729 | 730 | 770 |
| 231 | 269 | 993 | -937 | 827 | -671 | 476 | -255 | 019 | 218 | -443 | 642 | 731 | 769 |
| 232 | 268 | 994 | -943 | 844 | -703 | 525 | -321 | 100 | 125 | -345 | 546 | 732 | 768 |
| 233 | 267 | 994 | -949 | 861 | -733 | 572 | -386 | 181 | 031 | -243 | 443 | 733 | 767 |
| 234 | 266 | 995 | -955 | 876 | -762 | 618 | -448 | 261 | -063 | -138 | 333 | 734 | 766 |
| | | | | | | | | | | | | | |
| 235 | 265 | 996 | -960 | 891 | -790 | 661 | -509 | 339 | -156 | -031 | 218 | 735 | 765 |
| 236 | 264 | 996 | -965 | 905 | -816 | 703 | -567 | 414 | -249 | 075 | 100 | 736 | 764 |
| 237 | 263 | 997 | -970 | 918 | -841 | 742 | -623 | 487 | -339 | 181 | -019 | 737 | 763 |
| 238 | 262 | 997 | -975 | 930 | -864 | 778 | -675 | 557 | -426 | 285 | -138 | 738 | 762 |
| 239 | 261 | 998 | -979 | 941 | -885 | 813 | -725 | 623 | -509 | 386 | -255 | 739 | 761 |
| | | | | | | | | | | | | | |
| 240 | 260 | 998 | -982 | 951 | -905 | 844 | -771 | 685 | -588 | 482 | -368 | 740 | 760 |
| 241 | 259 | 998 | -986 | 960 | -923 | 873 | -813 | 742 | -661 | 572 | -476 | 741 | 759 |
| 242 | 258 | 999 | -989 | 969 | -939 | 899 | -851 | 794 | -729 | 657 | -578 | 742 | 758 |
| 243 | 257 | 999 | -991 | 976 | -953 | 923 | -885 | 841 | -790 | 733 | -671 | 743 | 757 |
| 244 | 256 | 999 | -994 | 982 | -965 | 943 | -915 | 882 | -844 | 802 | -754 | 744 | 756 |
| | | | | | | | | | | | | | |
| 245 | 255 | 1000 | -996 | 988 | -976 | 960 | -941 | 918 | -891 | 861 | -827 | 745 | 755 |
| 246 | 254 | 1000 | -997 | 992 | -985 | 975 | -962 | 947 | -930 | 910 | -888 | 746 | 754 |
| 247 | 253 | 1000 | -998 | 996 | -991 | 986 | -979 | 970 | -960 | 949 | -937 | 747 | 753 |
| 248 | 252 | 1000 | -999 | 998 | -996 | 994 | -990 | 987 | -982 | 977 | -972 | 748 | 752 |
| 249 | 251 | 1000 | -1000 | 1000 | -999 | 998 | -998 | 997 | -996 | 994 | -993 | 749 | 751 |
| | | | | | | | | | | | | | |
| 250 | 250 | 1000 | -1000 | 1000 | -1000 | 1000 | -1000 | 1000 | -1000 | 1000 | -1000 | 750 | 750 |

TABLE 8.5A (continued)

 $\sin 2\pi hx$ (h odd) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=21$ | 23 | 25 | 27 | 29 | 31 | 33 | 35 | 37 | 39 | Change sign.
x | |
|-----------------------|-----|--------|-------|-------|-------|------|-------|-------|-------|------|-------|---------------------|-----|
| 220 | 280 | −685 | 368 | 000 | −368 | 685 | −905 | 998 | −951 | 771 | −482 | 720 | 780 |
| 221 | 279 | −775 | 498 | −156 | −206 | 541 | −805 | 964 | −996 | 897 | −680 | 721 | 779 |
| 222 | 278 | −851 | 618 | −309 | −038 | 380 | −675 | 888 | −992 | 975 | −838 | 722 | 778 |
| 223 | 277 | −913 | 725 | −454 | 132 | 206 | −520 | 775 | −941 | 1000 | −945 | 723 | 777 |
| 224 | 276 | −959 | 816 | −588 | 297 | 025 | −345 | 628 | −844 | 972 | −996 | 724 | 776 |
| | | | | | | | | | | | | | |
| 225 | 275 | −988 | 891 | −707 | 454 | −156 | −156 | 454 | −707 | 891 | −988 | 725 | 775 |
| 226 | 274 | −1000 | 947 | −809 | 598 | −333 | 038 | 261 | −536 | 762 | −920 | 726 | 774 |
| 227 | 273 | −994 | 983 | −891 | 725 | −498 | 230 | 057 | −339 | 593 | −798 | 727 | 773 |
| 228 | 272 | −972 | 999 | −951 | 831 | −647 | 414 | −150 | −125 | 391 | −628 | 728 | 772 |
| 229 | 271 | −932 | 994 | −988 | 913 | −775 | 583 | −351 | 094 | 169 | −420 | 729 | 771 |
| | | | | | | | | | | | | | |
| 230 | 270 | −876 | 969 | −1000 | 969 | −876 | 729 | −536 | 309 | −063 | −187 | 730 | 770 |
| 231 | 269 | −805 | 923 | −988 | 997 | −949 | 848 | −698 | 509 | −291 | 057 | 731 | 769 |
| 232 | 268 | −720 | 858 | −951 | 996 | −990 | 934 | −831 | 685 | −504 | 297 | 732 | 768 |
| 233 | 267 | −623 | 775 | −891 | 967 | −999 | 986 | −927 | 827 | −689 | 520 | 733 | 767 |
| 234 | 266 | −514 | 675 | −809 | 910 | −975 | 1000 | −985 | 930 | −838 | 712 | 734 | 766 |
| | | | | | | | | | | | | | |
| 235 | 265 | −397 | 562 | −707 | 827 | −918 | 976 | −1000 | 988 | −941 | 861 | 735 | 765 |
| 236 | 264 | −273 | 437 | −588 | 720 | −831 | 915 | −972 | 998 | −994 | 959 | 736 | 764 |
| 237 | 263 | −144 | 303 | −454 | 593 | −716 | 820 | −902 | 960 | −993 | 999 | 737 | 763 |
| 238 | 262 | −013 | 163 | −309 | 448 | −578 | 694 | −794 | 876 | −939 | 980 | 738 | 762 |
| 239 | 261 | 119 | 019 | −156 | 291 | −420 | 541 | −652 | 750 | −834 | 902 | 739 | 761 |
| | | | | | | | | | | | | | |
| 240 | 260 | 249 | −125 | 000 | 125 | −249 | 368 | −482 | 588 | −685 | 771 | 740 | 760 |
| 241 | 259 | 374 | −267 | 156 | −044 | −069 | 181 | −291 | 397 | −498 | 593 | 741 | 759 |
| 242 | 258 | 493 | −403 | 309 | −212 | 113 | −013 | −088 | 187 | −285 | 380 | 742 | 758 |
| 243 | 257 | 603 | −531 | 454 | −374 | 291 | −206 | 119 | −031 | −057 | 144 | 743 | 757 |
| 244 | 256 | 703 | −647 | 588 | −525 | 460 | −391 | 321 | −249 | 175 | −100 | 744 | 756 |
| | | | | | | | | | | | | | |
| 245 | 255 | 790 | −750 | 707 | −661 | 613 | −562 | 509 | −454 | 397 | −339 | 745 | 755 |
| 246 | 254 | 864 | −838 | 809 | −778 | 746 | −712 | 675 | −637 | 598 | −557 | 746 | 754 |
| 247 | 253 | 923 | −907 | 891 | −873 | 854 | −834 | 813 | −790 | 767 | −742 | 747 | 753 |
| 248 | 252 | 965 | −959 | 951 | −943 | 934 | −925 | 915 | −905 | 894 | −882 | 748 | 752 |
| 249 | 251 | 991 | −990 | 988 | −986 | 983 | −981 | 979 | −976 | 973 | −970 | 749 | 751 |
| | | | | | | | | | | | | | |
| 250 | 250 | 1000 | −1000 | 1000 | −1000 | 1000 | −1000 | 1000 | −1000 | 1000 | −1000 | 750 | 750 |

TABLE 8.5B

 $\sin 2\pi hx$ (h even) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=2$ | 4 | 6 | 8 | 10 | 12 | 14 | 16 | 18 | 20 | Change sign.
x | |
|-----------------------|-----|-------|-----|------|------|------|------|------|------|------|------|---------------------|------|
| 000 | 500 | 000 | 000 | 000 | 000 | 000 | 000 | 000 | 000 | 000 | 000 | 500 | 1000 |
| 001 | 501 | 013 | 025 | 038 | 050 | 063 | 075 | 088 | 100 | 113 | 125 | 499 | 999 |
| 002 | 502 | 025 | 050 | 075 | 100 | 125 | 150 | 175 | 200 | 224 | 249 | 498 | 998 |
| 003 | 503 | 038 | 075 | 113 | 150 | 187 | 224 | 261 | 297 | 333 | 368 | 497 | 997 |
| 004 | 504 | 050 | 100 | 150 | 200 | 249 | 297 | 345 | 391 | 437 | 482 | 496 | 996 |
| 005 | 505 | 063 | 125 | 187 | 249 | 309 | 368 | 426 | 482 | 536 | 588 | 495 | 995 |
| 006 | 506 | 075 | 150 | 224 | 297 | 368 | 437 | 504 | 567 | 628 | 685 | 494 | 994 |
| 007 | 507 | 088 | 175 | 261 | 345 | 426 | 504 | 578 | 647 | 712 | 771 | 493 | 993 |
| 008 | 508 | 100 | 200 | 297 | 391 | 482 | 567 | 647 | 720 | 786 | 844 | 492 | 992 |
| 009 | 509 | 113 | 224 | 333 | 437 | 536 | 628 | 712 | 786 | 851 | 905 | 491 | 991 |
| 010 | 510 | 125 | 249 | 368 | 482 | 588 | 685 | 771 | 844 | 905 | 951 | 490 | 990 |
| 011 | 511 | 138 | 273 | 403 | 525 | 637 | 738 | 824 | 894 | 947 | 982 | 489 | 989 |
| 012 | 512 | 150 | 297 | 437 | 567 | 685 | 786 | 870 | 934 | 977 | 998 | 488 | 988 |
| 013 | 513 | 163 | 321 | 471 | 608 | 729 | 831 | 910 | 965 | 995 | 998 | 487 | 987 |
| 014 | 514 | 175 | 345 | 504 | 647 | 771 | 870 | 943 | 987 | 1000 | 982 | 486 | 986 |
| 015 | 515 | 187 | 368 | 536 | 685 | 809 | 905 | 969 | 998 | 992 | 951 | 485 | 985 |
| 016 | 516 | 200 | 391 | 567 | 720 | 844 | 934 | 987 | 999 | 972 | 905 | 484 | 984 |
| 017 | 517 | 212 | 414 | 598 | 754 | 876 | 959 | 997 | 990 | 939 | 844 | 483 | 983 |
| 018 | 518 | 224 | 437 | 628 | 786 | 905 | 977 | 1000 | 972 | 894 | 771 | 482 | 982 |
| 019 | 519 | 237 | 460 | 657 | 816 | 930 | 990 | 995 | 943 | 838 | 685 | 481 | 981 |
| 020 | 520 | 249 | 482 | 685 | 844 | 951 | 998 | 982 | 905 | 771 | 588 | 480 | 980 |
| 021 | 521 | 261 | 504 | 712 | 870 | 969 | 1000 | 962 | 858 | 694 | 482 | 479 | 979 |
| 022 | 522 | 273 | 525 | 738 | 894 | 982 | 996 | 934 | 802 | 608 | 368 | 478 | 978 |
| 023 | 523 | 285 | 546 | 762 | 915 | 992 | 987 | 899 | 738 | 514 | 249 | 477 | 977 |
| 024 | 524 | 297 | 567 | 786 | 934 | 998 | 972 | 858 | 666 | 414 | 125 | 476 | 976 |
| 025 | 525 | 309 | 588 | 809 | 951 | 1000 | 951 | 809 | 588 | 309 | 000 | 475 | 975 |
| 026 | 526 | 321 | 608 | 831 | 965 | 998 | 925 | 754 | 504 | 200 | -125 | 474 | 974 |
| 027 | 527 | 333 | 628 | 851 | 977 | 992 | 894 | 694 | 414 | 088 | -249 | 473 | 973 |
| 028 | 528 | 345 | 647 | 870 | 987 | 982 | 858 | 628 | 321 | -025 | -368 | 472 | 972 |
| 029 | 529 | 356 | 666 | 888 | 994 | 969 | 816 | 557 | 224 | -138 | -482 | 471 | 971 |
| 030 | 530 | 368 | 685 | 905 | 998 | 951 | 771 | 482 | 125 | -249 | -588 | 470 | 970 |
| 031 | 531 | 380 | 703 | 920 | 1000 | 930 | 720 | 403 | 025 | -356 | -685 | 469 | 969 |
| 032 | 532 | 391 | 720 | 934 | 999 | 905 | 666 | 321 | -075 | -460 | -771 | 468 | 968 |
| 033 | 533 | 403 | 738 | 947 | 996 | 876 | 608 | 237 | -175 | -557 | -844 | 467 | 967 |
| 034 | 534 | 414 | 754 | 959 | 990 | 844 | 546 | 150 | -273 | -647 | -905 | 466 | 966 |
| 035 | 535 | 426 | 771 | 969 | 982 | 809 | 482 | 063 | -368 | -729 | -951 | 465 | 965 |
| 036 | 536 | 437 | 786 | 977 | 972 | 771 | 414 | -025 | -460 | -802 | -982 | 464 | 964 |
| 037 | 537 | 448 | 802 | 985 | 959 | 729 | 345 | -113 | -546 | -864 | -998 | 463 | 963 |
| 038 | 538 | 460 | 816 | 990 | 943 | 685 | 273 | -200 | -628 | -915 | -998 | 462 | 962 |
| 039 | 539 | 471 | 831 | 995 | 925 | 637 | 200 | -285 | -703 | -955 | -982 | 461 | 961 |
| 040 | 540 | 482 | 844 | 998 | 905 | 588 | 125 | -368 | -771 | -982 | -951 | 460 | 960 |
| 041 | 541 | 493 | 858 | 1000 | 882 | 536 | 050 | -448 | -831 | -997 | -905 | 459 | 959 |
| 042 | 542 | 504 | 870 | 1000 | 858 | 482 | -025 | -525 | -882 | -999 | -844 | 458 | 958 |
| 043 | 543 | 514 | 882 | 999 | 831 | 426 | -100 | -590 | -925 | -989 | -771 | 457 | 957 |
| 044 | 544 | 525 | 894 | 996 | 802 | 368 | -175 | -666 | -959 | -965 | -685 | 456 | 956 |

TABLE 8.5B

 $\sin 2\pi hx$ (h even) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=22$ | 24 | 26 | 28 | 30 | 32 | 34 | 36 | 38 | 40 | Change sign.
x | |
|-----------------------|-----|--------|------|-------|------|-------|------|-------|------|------|------|---------------------|------|
| 000 | 500 | 000 | 000 | 000 | 000 | 000 | 000 | 000 | 000 | 000 | 000 | 500 | 1000 |
| 001 | 501 | 138 | 150 | 163 | 175 | 187 | 200 | 212 | 224 | 237 | 249 | 499 | 999 |
| 002 | 502 | 273 | 297 | 321 | 345 | 368 | 391 | 414 | 437 | 460 | 482 | 498 | 998 |
| 003 | 503 | 403 | 437 | 471 | 504 | 536 | 567 | 598 | 628 | 657 | 685 | 497 | 997 |
| 004 | 504 | 525 | 567 | 608 | 647 | 685 | 720 | 754 | 786 | 816 | 844 | 496 | 996 |
| | | | | | | | | | | | | | |
| 005 | 505 | 637 | 685 | 729 | 771 | 809 | 844 | 876 | 905 | 930 | 951 | 495 | 995 |
| 006 | 506 | 738 | 786 | 831 | 870 | 905 | 934 | 959 | 977 | 990 | 998 | 494 | 994 |
| 007 | 507 | 824 | 870 | 910 | 943 | 969 | 987 | 997 | 1000 | 995 | 982 | 493 | 993 |
| 008 | 508 | 894 | 934 | 965 | 987 | 998 | 999 | 990 | 972 | 943 | 905 | 492 | 992 |
| 009 | 509 | 947 | 977 | 995 | 1000 | 992 | 972 | 939 | 894 | 838 | 771 | 491 | 991 |
| | | | | | | | | | | | | | |
| 010 | 510 | 982 | 998 | 998 | 982 | 951 | 905 | 844 | 771 | 685 | 588 | 490 | 990 |
| 011 | 511 | 999 | 996 | 975 | 934 | 876 | 802 | 712 | 608 | 493 | 368 | 489 | 989 |
| 012 | 512 | 996 | 972 | 925 | 858 | 771 | 666 | 546 | 414 | 273 | 125 | 488 | 988 |
| 013 | 513 | 975 | 925 | 851 | 754 | 637 | 504 | 356 | 200 | 038 | -125 | 487 | 987 |
| 014 | 514 | 934 | 858 | 754 | 628 | 482 | 321 | 150 | -025 | -200 | -368 | 486 | 986 |
| | | | | | | | | | | | | | |
| 015 | 515 | 876 | 771 | 637 | 482 | 309 | 125 | -063 | -249 | -426 | -588 | 485 | 985 |
| 016 | 516 | 802 | 666 | 504 | 321 | 125 | -075 | -273 | -460 | -628 | -771 | 484 | 984 |
| 017 | 517 | 712 | 546 | 356 | 150 | -063 | -273 | -471 | -647 | -794 | -905 | 483 | 983 |
| 018 | 518 | 608 | 414 | 200 | -025 | -249 | -460 | -647 | -802 | -915 | -982 | 482 | 982 |
| 019 | 519 | 493 | 273 | 038 | -200 | -426 | -628 | -794 | -915 | -985 | -998 | 481 | 981 |
| | | | | | | | | | | | | | |
| 020 | 520 | 368 | 125 | -125 | -368 | -588 | -771 | -905 | -982 | -998 | -951 | 480 | 980 |
| 021 | 521 | 237 | -025 | -285 | -525 | -729 | -882 | -975 | -999 | -955 | -844 | 479 | 979 |
| 022 | 522 | 100 | -175 | -437 | -666 | -844 | -959 | -1000 | -965 | -858 | -685 | 478 | 978 |
| 023 | 523 | -038 | -321 | -578 | -786 | -930 | -996 | -980 | -882 | -712 | -482 | 477 | 977 |
| 024 | 524 | -175 | -460 | -703 | -882 | -982 | -994 | -915 | -754 | -525 | -249 | 476 | 976 |
| | | | | | | | | | | | | | |
| 025 | 525 | -309 | -588 | -809 | -951 | -1000 | -951 | -809 | -588 | -309 | 000 | 475 | 975 |
| 026 | 526 | -437 | -703 | -894 | -990 | -982 | -870 | -666 | -391 | -075 | 249 | 474 | 974 |
| 027 | 527 | -557 | -802 | -955 | -999 | -930 | -754 | -493 | -175 | 163 | 482 | 473 | 973 |
| 028 | 528 | -666 | -882 | -990 | -977 | -844 | -608 | -297 | 050 | 391 | 685 | 472 | 972 |
| 029 | 529 | -762 | -943 | -1000 | -925 | -729 | -437 | -088 | 273 | 598 | 844 | 471 | 971 |
| | | | | | | | | | | | | | |
| 030 | 530 | -844 | -982 | -982 | -844 | -588 | -249 | 125 | 482 | 771 | 951 | 470 | 970 |
| 031 | 531 | -910 | -999 | -939 | -738 | -426 | -050 | 333 | 666 | 899 | 998 | 469 | 969 |
| 032 | 532 | -959 | -994 | -870 | -608 | -249 | 150 | 525 | 816 | 977 | 982 | 468 | 968 |
| 033 | 533 | -989 | -965 | -778 | -460 | -063 | 345 | 694 | 925 | 1000 | 905 | 467 | 967 |
| 034 | 534 | -1000 | -915 | -666 | -297 | 125 | 525 | 831 | 987 | 965 | 771 | 466 | 966 |
| | | | | | | | | | | | | | |
| 035 | 535 | -992 | -844 | -536 | -125 | 309 | 685 | 930 | 998 | 876 | 588 | 465 | 965 |
| 036 | 536 | -965 | -754 | -391 | 050 | 482 | 816 | 987 | 959 | 738 | 368 | 464 | 964 |
| 037 | 537 | -920 | -647 | -237 | 224 | 637 | 915 | 999 | 870 | 557 | 125 | 463 | 963 |
| 038 | 538 | -858 | -525 | -075 | 391 | 771 | 977 | 965 | 738 | 345 | -125 | 462 | 962 |
| 039 | 539 | -778 | -391 | 088 | 546 | 876 | 1000 | 888 | 567 | 113 | -368 | 461 | 961 |
| | | | | | | | | | | | | | |
| 040 | 540 | -685 | -249 | 249 | 685 | 951 | 982 | 771 | 368 | -125 | -588 | 460 | 960 |
| 041 | 541 | -578 | -100 | 403 | 802 | 992 | 925 | 618 | 150 | -356 | -771 | 459 | 959 |
| 042 | 542 | -460 | 050 | 546 | 894 | 998 | 831 | 437 | -075 | -567 | -905 | 458 | 958 |
| 043 | 543 | -333 | 200 | 675 | 959 | 969 | 703 | 237 | -297 | -746 | -982 | 457 | 957 |
| 044 | 544 | -200 | 345 | 786 | 994 | 905 | 546 | 025 | -504 | -882 | -998 | 456 | 956 |

TABLE 8.5B (continued)

 $\sin 2\pi hx$ (h even) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=2$ | 4 | 6 | 8 | 10 | 12 | 14 | 16 | 18 | 20 | Change sign.
x | |
|-----------------------|-----|-------|------|------|------|-------|------|------|-------|------|------|---------------------|-----|
| 045 | 545 | 536 | 905 | 992 | 771 | 309 | -249 | -729 | -982 | -930 | -588 | 455 | 955 |
| 046 | 546 | 546 | 915 | 987 | 738 | 249 | -321 | -780 | -996 | -882 | -482 | 454 | 954 |
| 047 | 547 | 557 | 925 | 980 | 703 | 187 | -391 | -838 | -1000 | -824 | -368 | 453 | 953 |
| 048 | 548 | 567 | 934 | 972 | 666 | 125 | -460 | -882 | -994 | -754 | -249 | 452 | 952 |
| 049 | 549 | 578 | 943 | 962 | 628 | 063 | -525 | -920 | -977 | -675 | -125 | 451 | 951 |
| 050 | 550 | 588 | 951 | 951 | 588 | 000 | -588 | -951 | -951 | -588 | 000 | 450 | 950 |
| 051 | 551 | 598 | 959 | 939 | 546 | -063 | -647 | -975 | -915 | -493 | 125 | 449 | 949 |
| 052 | 552 | 608 | 965 | 925 | 504 | -125 | -703 | -990 | -870 | -391 | 249 | 448 | 948 |
| 053 | 553 | 618 | 972 | 910 | 460 | -187 | -754 | -999 | -816 | -285 | 368 | 447 | 947 |
| 054 | 554 | 628 | 977 | 894 | 414 | -249 | -802 | -999 | -754 | -175 | 482 | 446 | 946 |
| 055 | 555 | 637 | 982 | 876 | 368 | -309 | -844 | -992 | -685 | -063 | 588 | 445 | 945 |
| 056 | 556 | 647 | 987 | 858 | 321 | -368 | -882 | -977 | -608 | 050 | 685 | 444 | 944 |
| 057 | 557 | 657 | 990 | 838 | 273 | -426 | -915 | -955 | -525 | 163 | 771 | 443 | 943 |
| 058 | 558 | 666 | 994 | 816 | 224 | -482 | -943 | -925 | -437 | 273 | 844 | 442 | 942 |
| 059 | 559 | 675 | 996 | 794 | 175 | -536 | -965 | -888 | -345 | 380 | 905 | 441 | 941 |
| 060 | 560 | 685 | 998 | 771 | 125 | -588 | -982 | -844 | -249 | 482 | 951 | 440 | 940 |
| 061 | 561 | 694 | 999 | 746 | 075 | -637 | -994 | -794 | -150 | 578 | 982 | 439 | 939 |
| 062 | 562 | 703 | 1000 | 720 | 025 | -685 | -999 | -738 | -050 | 666 | 998 | 438 | 938 |
| 063 | 563 | 712 | 1000 | 694 | -025 | -729 | -999 | -675 | 050 | 746 | 998 | 437 | 937 |
| 064 | 564 | 720 | 999 | 666 | -075 | -771 | -994 | -608 | 150 | 816 | 982 | 436 | 936 |
| 065 | 565 | 729 | 998 | 637 | -125 | -809 | -982 | -536 | 249 | 876 | 951 | 435 | 935 |
| 066 | 566 | 738 | 996 | 608 | -175 | -844 | -965 | -460 | 345 | 925 | 905 | 434 | 934 |
| 067 | 567 | 746 | 994 | 578 | -224 | -876 | -943 | -380 | 437 | 962 | 844 | 433 | 933 |
| 068 | 568 | 754 | 990 | 546 | -273 | -905 | -915 | -297 | 525 | 987 | 771 | 432 | 932 |
| 069 | 569 | 762 | 987 | 514 | -321 | -930 | -882 | -212 | 608 | 999 | 685 | 431 | 931 |
| 070 | 570 | 771 | 982 | 482 | -368 | -951 | -844 | -125 | 685 | 998 | 588 | 430 | 930 |
| 071 | 571 | 778 | 977 | 448 | -414 | -969 | -802 | -038 | 754 | 985 | 482 | 429 | 929 |
| 072 | 572 | 786 | 972 | 414 | -460 | -982 | -754 | 050 | 816 | 959 | 368 | 428 | 928 |
| 073 | 573 | 794 | 965 | 380 | -504 | -992 | -703 | 138 | 870 | 920 | 249 | 427 | 927 |
| 074 | 574 | 802 | 959 | 345 | -546 | -998 | -647 | 224 | 915 | 870 | 125 | 426 | 926 |
| 075 | 575 | 809 | 951 | 309 | -588 | -1000 | -588 | 309 | 951 | 809 | 000 | 425 | 925 |
| 076 | 576 | 816 | 943 | 273 | -628 | -998 | -525 | 391 | 977 | 738 | -125 | 424 | 924 |
| 077 | 577 | 824 | 934 | 237 | -666 | -992 | -460 | 471 | 994 | 657 | -249 | 423 | 923 |
| 078 | 578 | 831 | 925 | 200 | -703 | -982 | -391 | 546 | 1000 | 567 | -368 | 422 | 922 |
| 079 | 579 | 838 | 915 | 163 | -738 | -969 | -321 | 618 | 996 | 471 | -482 | 421 | 921 |
| 080 | 580 | 844 | 905 | 125 | -771 | -951 | -249 | 685 | 982 | 368 | -588 | 420 | 920 |
| 081 | 581 | 851 | 894 | 088 | -802 | -930 | -175 | 746 | 959 | 261 | -685 | 419 | 919 |
| 082 | 582 | 858 | 882 | 050 | -831 | -905 | -100 | 802 | 925 | 150 | -771 | 418 | 918 |
| 083 | 583 | 864 | 870 | 013 | -858 | -876 | -025 | 851 | 882 | 038 | -844 | 417 | 917 |
| 084 | 584 | 870 | 858 | -025 | -882 | -844 | 050 | 894 | 831 | -075 | -905 | 416 | 916 |
| 085 | 585 | 876 | 844 | -063 | -905 | -809 | 125 | 930 | 771 | -187 | -951 | 415 | 915 |
| 086 | 586 | 882 | 831 | -100 | -925 | -771 | 200 | 959 | 703 | -297 | -982 | 414 | 914 |
| 087 | 587 | 888 | 816 | -138 | -943 | -729 | 273 | 980 | 628 | -403 | -998 | 413 | 913 |
| 088 | 588 | 894 | 802 | -175 | -959 | -685 | 345 | 994 | 546 | -504 | -998 | 412 | 912 |
| 089 | 589 | 899 | 786 | -212 | -972 | -637 | 414 | 1000 | 460 | -598 | -982 | 411 | 911 |

TABLE 8.5B (continued)

 $\sin 2\pi hx$ (h even) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=22$ | 24 | 26 | 28 | 30 | 32 | 34 | 36 | 38 | 40 | Change sign.
x | |
|-----------------------|-----|--------|-------|------|------|------|-------|-------|------|-------|------|---------------------|-----|
| 045 | 545 | -063 | 482 | 876 | 998 | 809 | 368 | -187 | -685 | -969 | -951 | 455 | 955 |
| 046 | 546 | 075 | 608 | 943 | 972 | 685 | 175 | -391 | -831 | -1000 | -844 | 454 | 954 |
| 047 | 547 | 212 | 720 | 985 | 915 | 536 | -025 | -578 | -934 | -975 | -685 | 453 | 953 |
| 048 | 548 | 345 | 816 | 1000 | 831 | 368 | -224 | -738 | -990 | -894 | -482 | 452 | 952 |
| 049 | 549 | 471 | 894 | 989 | 720 | 187 | -414 | -864 | -996 | -762 | -249 | 451 | 951 |
| | | | | | | | | | | | | | |
| 050 | 550 | 588 | 951 | 951 | 588 | 000 | -588 | -951 | -951 | -588 | 000 | 450 | 950 |
| 051 | 551 | 694 | 987 | 888 | 437 | -187 | -738 | -995 | -858 | -380 | 249 | 449 | 949 |
| 052 | 552 | 786 | 1000 | 802 | 273 | -368 | -858 | -994 | -720 | -150 | 482 | 448 | 948 |
| 053 | 553 | 864 | 990 | 694 | 100 | -536 | -943 | -947 | -546 | 088 | 685 | 447 | 947 |
| 054 | 554 | 925 | 959 | 567 | -075 | -685 | -990 | -858 | -345 | 321 | 844 | 446 | 946 |
| | | | | | | | | | | | | | |
| 055 | 555 | 969 | 905 | 426 | -249 | -809 | -998 | -729 | -125 | 536 | 951 | 445 | 945 |
| 056 | 556 | 994 | 831 | 273 | -414 | -905 | -965 | -567 | 100 | 720 | 998 | 444 | 944 |
| 057 | 557 | 1000 | 738 | 113 | -567 | -969 | -894 | -380 | 321 | 864 | 982 | 443 | 943 |
| 058 | 558 | 987 | 628 | -050 | -703 | -998 | -786 | -175 | 525 | 959 | 905 | 442 | 942 |
| 059 | 559 | 955 | 504 | -212 | -816 | -992 | -647 | 038 | 703 | 999 | 771 | 441 | 941 |
| | | | | | | | | | | | | | |
| 060 | 560 | 905 | 368 | -368 | -905 | -951 | -482 | 249 | 844 | 982 | 588 | 440 | 940 |
| 061 | 561 | 838 | 224 | -514 | -965 | -876 | -297 | 448 | 943 | 910 | 368 | 439 | 939 |
| 062 | 562 | 754 | 075 | -647 | -996 | -771 | -100 | 628 | 994 | 786 | 125 | 438 | 938 |
| 063 | 563 | 657 | -075 | -762 | -996 | -637 | 100 | 778 | 994 | 618 | -125 | 437 | 937 |
| 064 | 564 | 546 | -224 | -858 | -965 | -482 | 297 | 894 | 943 | 414 | -368 | 436 | 936 |
| | | | | | | | | | | | | | |
| 065 | 565 | 426 | -368 | -930 | -905 | -309 | 482 | 969 | 844 | 187 | -588 | 435 | 935 |
| 066 | 566 | 297 | -504 | -977 | -816 | -125 | 647 | 999 | 703 | -050 | -771 | 434 | 934 |
| 067 | 567 | 163 | -628 | -999 | -703 | 063 | 786 | 985 | 525 | -285 | -905 | 433 | 933 |
| 068 | 568 | 025 | -738 | -994 | -567 | 249 | 894 | 925 | 321 | -504 | -982 | 432 | 932 |
| 069 | 569 | -113 | -831 | -962 | -414 | 426 | 965 | 824 | 100 | -694 | -998 | 431 | 931 |
| | | | | | | | | | | | | | |
| 070 | 570 | -249 | -905 | -905 | -249 | 588 | 998 | 685 | -125 | -844 | -951 | 430 | 930 |
| 071 | 571 | -380 | -959 | -824 | -075 | 729 | 990 | 514 | -345 | -947 | -844 | 429 | 929 |
| 072 | 572 | -504 | -990 | -720 | 100 | 844 | 943 | 321 | -546 | -996 | -685 | 428 | 928 |
| 073 | 573 | -618 | -1000 | -598 | 273 | 930 | 858 | 113 | -720 | -989 | -482 | 427 | 927 |
| 074 | 574 | -720 | -987 | -460 | 437 | 982 | 738 | -100 | -858 | -925 | -249 | 426 | 926 |
| | | | | | | | | | | | | | |
| 075 | 575 | -809 | -951 | -309 | 588 | 1000 | 588 | -309 | -951 | -809 | 000 | 425 | 925 |
| 076 | 576 | -882 | -894 | -150 | 720 | 982 | 414 | -504 | -996 | -647 | 249 | 424 | 924 |
| 077 | 577 | -939 | -816 | 013 | 831 | 930 | 224 | -675 | -990 | -448 | 482 | 423 | 923 |
| 078 | 578 | -977 | -720 | 175 | 915 | 844 | 025 | -816 | -934 | -224 | 685 | 422 | 922 |
| 079 | 579 | -997 | -608 | 333 | 972 | 729 | -175 | -920 | -831 | 013 | 844 | 421 | 921 |
| | | | | | | | | | | | | | |
| 080 | 580 | -998 | -482 | 482 | 998 | 588 | -368 | -982 | -685 | 249 | 951 | 420 | 920 |
| 081 | 581 | -980 | -345 | 618 | 994 | 426 | -546 | -1000 | -504 | 471 | 998 | 419 | 919 |
| 082 | 582 | -943 | -200 | 738 | 959 | 249 | -703 | -972 | -297 | 666 | 982 | 418 | 918 |
| 083 | 583 | -888 | -050 | 838 | 894 | 063 | -831 | -899 | -075 | 824 | 905 | 417 | 917 |
| 084 | 584 | -816 | 100 | 915 | 802 | -125 | -925 | -786 | 150 | 934 | 771 | 416 | 916 |
| | | | | | | | | | | | | | |
| 085 | 585 | -729 | 249 | 969 | 685 | -309 | -982 | -637 | 368 | 992 | 588 | 415 | 915 |
| 086 | 586 | -628 | 391 | 996 | 546 | -482 | -1000 | -460 | 567 | 994 | 368 | 414 | 914 |
| 087 | 587 | -514 | 525 | 997 | 391 | -637 | -977 | -261 | 738 | 939 | 125 | 413 | 913 |
| 088 | 588 | -391 | 647 | 972 | 224 | -771 | -915 | -050 | 870 | 831 | -125 | 412 | 912 |
| 089 | 589 | -261 | 754 | 920 | 050 | -876 | -816 | 163 | 959 | 675 | -368 | 411 | 911 |

TABLE 8.5B (*continued*)
 $\sin 2\pi hx$ (h even) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=2$ | 4 | 6 | 8 | 10 | 12 | 14 | 16 | 18 | 20 | Change sign.
x | |
|-----------------------|-----|-------|------|-------|-------|------|------|-------|------|-------|------|---------------------|-----|
| 090 | 590 | 905 | 771 | -249 | -982 | -588 | 482 | 990 | 368 | -685 | -951 | 410 | 910 |
| 091 | 591 | 910 | 754 | -285 | -990 | -536 | 546 | 989 | 273 | -762 | -905 | 409 | 909 |
| 092 | 592 | 915 | 738 | -321 | -996 | -482 | 608 | 962 | 175 | -831 | -844 | 408 | 908 |
| 093 | 593 | 920 | 720 | -356 | -999 | -426 | 666 | 947 | 075 | -888 | -771 | 407 | 907 |
| 094 | 594 | 925 | 703 | -391 | -1000 | -368 | 720 | 915 | -025 | -934 | -685 | 406 | 906 |
| | | | | | | | | | | | | | |
| 095 | 595 | 930 | 685 | -426 | -998 | -309 | 771 | 876 | -125 | -969 | -588 | 405 | 905 |
| 096 | 596 | 934 | 666 | -460 | -994 | -249 | 816 | 831 | -224 | -990 | -482 | 404 | 904 |
| 097 | 597 | 939 | 647 | -493 | -987 | -187 | 858 | 778 | -321 | -1000 | -368 | 403 | 903 |
| 098 | 598 | 943 | 628 | -525 | -977 | -125 | 894 | 720 | -414 | -996 | -249 | 402 | 902 |
| 099 | 599 | 947 | 608 | -557 | -965 | -063 | 925 | 657 | -504 | -980 | -125 | 401 | 901 |
| | | | | | | | | | | | | | |
| 100 | 600 | 951 | 588 | -588 | -951 | 000 | 951 | 588 | -588 | -951 | 000 | 400 | 900 |
| 101 | 601 | 955 | 567 | -618 | -934 | 063 | 972 | 514 | -666 | -910 | 125 | 399 | 899 |
| 102 | 602 | 959 | 546 | -647 | -915 | 125 | 987 | 437 | -738 | -858 | 249 | 398 | 898 |
| 103 | 603 | 962 | 525 | -675 | -894 | 187 | 996 | 356 | -802 | -794 | 368 | 397 | 897 |
| 104 | 604 | 965 | 504 | -703 | -870 | 249 | 1000 | 273 | -858 | -720 | 482 | 396 | 896 |
| | | | | | | | | | | | | | |
| 105 | 605 | 969 | 482 | -729 | -844 | 309 | 998 | 187 | -905 | -637 | 588 | 395 | 895 |
| 106 | 606 | 972 | 460 | -754 | -816 | 368 | 990 | 100 | -943 | -546 | 685 | 394 | 894 |
| 107 | 607 | 975 | 437 | -778 | -786 | 426 | 977 | 013 | -972 | -448 | 771 | 393 | 893 |
| 108 | 608 | 977 | 414 | -802 | -754 | 482 | 959 | -075 | -990 | -345 | 844 | 392 | 892 |
| 109 | 609 | 980 | 391 | -824 | -720 | 536 | 934 | -163 | -999 | -237 | 905 | 391 | 891 |
| | | | | | | | | | | | | | |
| 110 | 610 | 982 | 368 | -844 | -685 | 588 | 905 | -249 | -998 | -125 | 951 | 390 | 890 |
| 111 | 611 | 985 | 345 | -864 | -647 | 637 | 870 | -333 | -987 | -013 | 982 | 389 | 889 |
| 112 | 612 | 987 | 321 | -882 | -608 | 685 | 831 | -414 | -965 | 100 | 998 | 388 | 888 |
| 113 | 613 | 989 | 297 | -899 | -567 | 729 | 786 | -493 | -934 | 212 | 998 | 387 | 887 |
| 114 | 614 | 990 | 273 | -915 | -525 | 771 | 738 | -567 | -894 | 321 | 982 | 386 | 886 |
| | | | | | | | | | | | | | |
| 115 | 615 | 992 | 249 | -930 | -482 | 809 | 685 | -637 | -844 | 426 | 951 | 385 | 885 |
| 116 | 616 | 994 | 224 | -943 | -437 | 844 | 628 | -703 | -786 | 525 | 905 | 384 | 884 |
| 117 | 617 | 995 | 200 | -955 | -391 | 876 | 567 | -762 | -720 | 618 | 844 | 383 | 883 |
| 118 | 618 | 996 | 175 | -965 | -345 | 905 | 504 | -816 | -647 | 703 | 771 | 382 | 882 |
| 119 | 619 | 997 | 150 | -975 | -297 | 930 | 437 | -864 | -567 | 778 | 685 | 381 | 881 |
| | | | | | | | | | | | | | |
| 120 | 620 | 998 | 125 | -982 | -249 | 951 | 368 | -905 | -482 | 844 | 588 | 380 | 880 |
| 121 | 621 | 999 | 100 | -989 | -200 | 969 | 297 | -939 | -391 | 899 | 482 | 379 | 879 |
| 122 | 622 | 999 | 075 | -994 | -150 | 982 | 224 | -965 | -297 | 943 | 368 | 378 | 878 |
| 123 | 623 | 1000 | 050 | -997 | -100 | 992 | 150 | -985 | -200 | 975 | 249 | 377 | 877 |
| 124 | 624 | 1000 | 025 | -999 | -050 | 998 | 075 | -996 | -100 | 994 | 125 | 376 | 876 |
| | | | | | | | | | | | | | |
| 125 | 625 | 1000 | 000 | -1000 | 000 | 1000 | 000 | -1000 | 000 | 1000 | 000 | 375 | 875 |
| 126 | 626 | 1000 | -025 | -999 | 050 | 998 | -075 | -996 | 100 | 994 | -125 | 374 | 874 |
| 127 | 627 | 1000 | -050 | -997 | 100 | 992 | -150 | -985 | 200 | 975 | -249 | 373 | 873 |
| 128 | 628 | 999 | -075 | -994 | 150 | 982 | -224 | -965 | 297 | 943 | -368 | 372 | 872 |
| 129 | 629 | 999 | -100 | -989 | 200 | 969 | -297 | -939 | 391 | 899 | -482 | 371 | 871 |
| | | | | | | | | | | | | | |
| 130 | 630 | 998 | -125 | -982 | 249 | 951 | -368 | -905 | 482 | 844 | -588 | 370 | 870 |
| 131 | 631 | 997 | -150 | -975 | 297 | 930 | -437 | -864 | 567 | 778 | -685 | 369 | 869 |
| 132 | 632 | 996 | -175 | -965 | 345 | 905 | -504 | -816 | 647 | 703 | -771 | 368 | 868 |
| 133 | 633 | 995 | -200 | -955 | 391 | 876 | -567 | -762 | 720 | 618 | -844 | 367 | 867 |
| 134 | 634 | 994 | -224 | -943 | 437 | 844 | -628 | -703 | 786 | 525 | -905 | 366 | 866 |

TABLE 8.5B (continued)

 $\sin 2\pi hx$ (h even) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=22$ | 24 | 26 | 28 | 30 | 32 | 34 | 36 | 38 | 40 | Change sign.
x | |
|-----------------------|-----|--------|------|------|-------|-------|------|------|-------|-------|------|---------------------|-----|
| 090 | 590 | -125 | 844 | 844 | -125 | -951 | -685 | 368 | 998 | 482 | -588 | 410 | 910 |
| 091 | 591 | 013 | 915 | 746 | -297 | -992 | -525 | 557 | 987 | 261 | -771 | 409 | 909 |
| 092 | 592 | 150 | 965 | 628 | -460 | -998 | -345 | 720 | 925 | 025 | -905 | 408 | 908 |
| 093 | 593 | 285 | 994 | 493 | -608 | -969 | -150 | 851 | 816 | -212 | -982 | 407 | 907 |
| 094 | 594 | 414 | 999 | 345 | -738 | -905 | 050 | 943 | 666 | -437 | -998 | 406 | 906 |
| | | | | | | | | | | | | | |
| 095 | 595 | 536 | 982 | 187 | -844 | -809 | 249 | 992 | 482 | -637 | -951 | 405 | 905 |
| 096 | 596 | 647 | 943 | 025 | -925 | -685 | 437 | 996 | 273 | -802 | -844 | 404 | 904 |
| 097 | 597 | 746 | 882 | -138 | -977 | -536 | 608 | 955 | 050 | -920 | -685 | 403 | 903 |
| 098 | 598 | 831 | 802 | -297 | -999 | -368 | 754 | 870 | -175 | -987 | -482 | 402 | 902 |
| 099 | 599 | 899 | 703 | -448 | -990 | -187 | 870 | 746 | -391 | -997 | -249 | 401 | 901 |
| | | | | | | | | | | | | | |
| 100 | 600 | 951 | 588 | -588 | -951 | 000 | 951 | 588 | -588 | -951 | 000 | 400 | 900 |
| 101 | 601 | 985 | 460 | -712 | -882 | 187 | 994 | 403 | -754 | -851 | 249 | 399 | 899 |
| 102 | 602 | 999 | 321 | -816 | -786 | 368 | 996 | 200 | -882 | -703 | 482 | 398 | 898 |
| 103 | 603 | 995 | 175 | -899 | -666 | 536 | 959 | -013 | -965 | -514 | 685 | 397 | 897 |
| 104 | 604 | 972 | 025 | -959 | -525 | 685 | 882 | -224 | -999 | -297 | 844 | 396 | 896 |
| | | | | | | | | | | | | | |
| 105 | 605 | 930 | -125 | -992 | -368 | 809 | 771 | -426 | -982 | -063 | 951 | 395 | 895 |
| 106 | 606 | 870 | -273 | -999 | -200 | 905 | 628 | -608 | -915 | 175 | 998 | 394 | 894 |
| 107 | 607 | 794 | -414 | -980 | -025 | 969 | 460 | -762 | -802 | 403 | 982 | 393 | 893 |
| 108 | 608 | 703 | -546 | -934 | 150 | 998 | 273 | -882 | -647 | 608 | 905 | 392 | 892 |
| 109 | 609 | 598 | -666 | -864 | 321 | 992 | 075 | -962 | -460 | 778 | 771 | 391 | 891 |
| | | | | | | | | | | | | | |
| 110 | 610 | 482 | -771 | -771 | 482 | 951 | -125 | -998 | -249 | 905 | 588 | 390 | 890 |
| 111 | 611 | 356 | -858 | -657 | 628 | 876 | -321 | -989 | -025 | 980 | 368 | 389 | 889 |
| 112 | 612 | 224 | -925 | -525 | 754 | 771 | -504 | -934 | 200 | 999 | 125 | 388 | 888 |
| 113 | 613 | 088 | -972 | -380 | 858 | 637 | -666 | -838 | 414 | 962 | -125 | 387 | 887 |
| 114 | 614 | -050 | -996 | -224 | 934 | 482 | -802 | -703 | 608 | 870 | -368 | 386 | 886 |
| | | | | | | | | | | | | | |
| 115 | 615 | -187 | -998 | -063 | 982 | 309 | -905 | -536 | 771 | 729 | -588 | 385 | 885 |
| 116 | 616 | -321 | -977 | 100 | 1000 | 125 | -972 | -345 | 894 | 546 | -771 | 384 | 884 |
| 117 | 617 | -448 | -934 | 261 | 987 | -063 | -999 | -138 | 972 | 333 | -905 | 383 | 883 |
| 118 | 618 | -567 | -870 | 414 | 943 | -249 | -987 | 075 | 1000 | 100 | -982 | 382 | 882 |
| 119 | 619 | -675 | -786 | 557 | 870 | -426 | -934 | 285 | 977 | -138 | -998 | 381 | 881 |
| | | | | | | | | | | | | | |
| 120 | 620 | -771 | -685 | 685 | 771 | -588 | -844 | 482 | 905 | -368 | -951 | 380 | 880 |
| 121 | 621 | -851 | -567 | 794 | 647 | -729 | -720 | 657 | 786 | -578 | -844 | 379 | 879 |
| 122 | 622 | -915 | -437 | 882 | 504 | -844 | -567 | 802 | 628 | -754 | -685 | 378 | 878 |
| 123 | 623 | -962 | -297 | 947 | 345 | -930 | -391 | 910 | 437 | -888 | -482 | 377 | 877 |
| 124 | 624 | -990 | -150 | 987 | 175 | -982 | -200 | 977 | 224 | -972 | -249 | 376 | 876 |
| | | | | | | | | | | | | | |
| 125 | 625 | -1000 | 000 | 1000 | 000 | -1000 | 000 | 1000 | 000 | -1000 | 000 | 375 | 875 |
| 126 | 626 | -990 | 150 | 987 | -175 | -982 | 200 | 977 | -224 | -972 | 249 | 374 | 874 |
| 127 | 627 | -962 | 297 | 947 | -345 | -930 | 391 | 910 | -437 | -888 | 482 | 373 | 873 |
| 128 | 628 | -915 | 437 | 882 | -504 | -844 | 567 | 802 | -628 | -754 | 685 | 372 | 872 |
| 129 | 629 | -851 | 567 | 794 | -647 | -729 | 720 | 657 | -786 | -578 | 844 | 371 | 871 |
| | | | | | | | | | | | | | |
| 130 | 630 | -771 | 685 | 685 | -771 | -588 | 844 | 482 | -905 | -368 | 951 | 370 | 870 |
| 131 | 631 | -675 | 786 | 557 | -870 | -426 | 934 | 285 | -977 | -138 | 998 | 369 | 869 |
| 132 | 632 | -567 | 870 | 414 | -943 | -249 | 987 | 075 | -1000 | 100 | 982 | 368 | 868 |
| 133 | 633 | -448 | 934 | 261 | -987 | -063 | 999 | -138 | -972 | 333 | 905 | 367 | 867 |
| 134 | 634 | -321 | 977 | 100 | -1000 | 125 | 972 | -345 | -894 | 546 | 771 | 366 | 866 |

TABLE 8.5B (continued)
 $\sin 2\pi hx$ (h even) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=2$ | 4 | 6 | 8 | 10 | 12 | 14 | 16 | 18 | 20 | Change sign.
x | |
|-----------------------|-----|-------|------|------|------|-------|-------|------|-------|-------|------|---------------------|-----|
| 135 | 635 | 992 | -249 | -930 | 482 | 809 | -685 | -637 | 844 | 426 | -951 | 365 | 865 |
| 136 | 636 | 990 | -273 | -915 | 525 | 771 | -738 | -567 | 894 | 321 | -982 | 364 | 864 |
| 137 | 637 | 989 | -297 | -899 | 567 | 729 | -786 | -493 | 934 | 212 | -998 | 363 | 863 |
| 138 | 638 | 987 | -321 | -882 | 608 | 685 | -831 | -414 | 965 | 100 | -998 | 362 | 862 |
| 139 | 639 | 985 | -345 | -864 | 647 | 637 | -870 | -333 | 987 | -013 | -982 | 361 | 861 |
| | | | | | | | | | | | | | |
| 140 | 640 | 982 | -368 | -844 | 685 | 588 | -905 | -249 | 998 | -125 | -951 | 360 | 860 |
| 141 | 641 | 980 | -391 | -824 | 720 | 536 | -934 | -163 | 999 | -237 | -905 | 359 | 859 |
| 142 | 642 | 977 | -414 | -802 | 754 | 482 | -959 | -075 | 990 | -345 | -844 | 358 | 858 |
| 143 | 643 | 975 | -437 | -778 | 786 | 426 | -977 | 013 | 972 | -448 | -771 | 357 | 857 |
| 144 | 644 | 972 | -460 | -754 | 816 | 368 | -990 | 100 | 943 | -546 | -685 | 356 | 856 |
| | | | | | | | | | | | | | |
| 145 | 645 | 969 | -482 | -729 | 844 | 309 | -998 | 187 | 905 | -637 | -588 | 355 | 855 |
| 146 | 646 | 965 | -504 | -703 | 870 | 249 | -1000 | 273 | 858 | -720 | -482 | 354 | 854 |
| 147 | 647 | 962 | -525 | -675 | 894 | 187 | -996 | 356 | 802 | -794 | -368 | 353 | 853 |
| 148 | 648 | 959 | -546 | -647 | 915 | 125 | -987 | 437 | 738 | -858 | -249 | 352 | 852 |
| 149 | 649 | 955 | -567 | -618 | 934 | 063 | -972 | 514 | 666 | -910 | -125 | 351 | 851 |
| | | | | | | | | | | | | | |
| 150 | 650 | 951 | -588 | -588 | 951 | 000 | -951 | 588 | 588 | -951 | 000 | 350 | 850 |
| 151 | 651 | 947 | -608 | -557 | 965 | -063 | -925 | 657 | 504 | -980 | 125 | 349 | 849 |
| 152 | 652 | 943 | -628 | -525 | 977 | -125 | -894 | 720 | 414 | -996 | 249 | 348 | 848 |
| 153 | 653 | 939 | -647 | -493 | 987 | -187 | -858 | 778 | 321 | -1000 | 368 | 347 | 847 |
| 154 | 654 | 934 | -666 | -460 | 994 | -249 | -816 | 831 | 224 | -990 | 482 | 346 | 846 |
| | | | | | | | | | | | | | |
| 155 | 655 | 930 | -685 | -426 | 998 | -309 | -771 | 876 | 125 | -969 | 588 | 345 | 845 |
| 156 | 656 | 925 | -703 | -391 | 1000 | -368 | -720 | 915 | 025 | -934 | 685 | 344 | 844 |
| 157 | 657 | 920 | -720 | -356 | 999 | -426 | -666 | 947 | -075 | -888 | 771 | 343 | 843 |
| 158 | 658 | 915 | -738 | -321 | 996 | -482 | -608 | 972 | -175 | -831 | 844 | 342 | 842 |
| 159 | 659 | 910 | -754 | -285 | 990 | -536 | -546 | 989 | -273 | -762 | 905 | 341 | 841 |
| | | | | | | | | | | | | | |
| 160 | 660 | 905 | -771 | -249 | 982 | -588 | -482 | 998 | -368 | -685 | 951 | 340 | 840 |
| 161 | 661 | 899 | -786 | -212 | 972 | -637 | -414 | 1000 | -460 | -598 | 982 | 339 | 839 |
| 162 | 662 | 894 | -802 | -175 | 959 | -685 | -345 | 994 | -546 | -504 | 998 | 338 | 838 |
| 163 | 663 | 888 | -816 | -138 | 943 | -729 | -273 | 980 | -628 | -403 | 998 | 337 | 837 |
| 164 | 664 | 882 | -831 | -100 | 925 | -771 | -200 | 959 | -703 | -297 | 982 | 336 | 836 |
| | | | | | | | | | | | | | |
| 165 | 665 | 876 | -844 | -063 | 905 | -809 | -125 | 930 | -771 | -187 | 951 | 335 | 835 |
| 166 | 666 | 870 | -858 | -025 | 882 | -844 | -050 | 894 | -831 | -075 | 905 | 334 | 834 |
| 167 | 667 | 864 | -870 | 013 | 858 | -876 | 025 | 851 | -882 | 038 | 844 | 333 | 833 |
| 168 | 668 | 858 | -882 | 050 | 831 | -905 | 100 | 802 | -925 | 150 | 771 | 332 | 832 |
| 169 | 669 | 851 | -894 | 088 | 802 | -930 | 175 | 746 | -959 | 261 | 685 | 331 | 831 |
| | | | | | | | | | | | | | |
| 170 | 670 | 844 | -905 | 125 | 771 | -951 | 249 | 685 | -982 | 368 | 588 | 330 | 830 |
| 171 | 671 | 838 | -915 | 163 | 738 | -969 | 321 | 618 | -996 | 471 | 482 | 329 | 829 |
| 172 | 672 | 831 | -925 | 200 | 703 | -982 | 391 | 546 | -1000 | 567 | 368 | 328 | 828 |
| 173 | 673 | 824 | -934 | 237 | 666 | -992 | 460 | 471 | -994 | 657 | 249 | 327 | 827 |
| 174 | 674 | 816 | -943 | 273 | 628 | -998 | 525 | 391 | -977 | 738 | 125 | 326 | 826 |
| | | | | | | | | | | | | | |
| 175 | 675 | 809 | -951 | 309 | 588 | -1000 | 588 | 309 | -951 | 809 | 000 | 325 | 825 |
| 176 | 676 | 802 | -959 | 345 | 546 | -998 | 647 | 224 | -915 | 870 | -125 | 324 | 824 |
| 177 | 677 | 794 | -965 | 380 | 504 | -992 | 703 | 138 | -870 | 920 | -249 | 323 | 823 |
| 178 | 678 | 786 | -972 | 414 | 460 | -982 | 754 | 050 | -816 | 959 | -368 | 322 | 822 |
| 179 | 679 | 778 | -977 | 448 | 414 | -969 | 802 | -038 | -754 | 985 | -482 | 321 | 821 |

TABLE 8.5B (*continued*)
 $\sin 2\pi hx$ (h even) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=22$ | 24 | 26 | 28 | 30 | 32 | 34 | 36 | 38 | 40 | Change sign.
x | |
|-----------------------|-----|--------|------|------|------|------|------|-------|------|------|------|---------------------|-----|
| 135 | 635 | −187 | 998 | −063 | −982 | 309 | 905 | −536 | −771 | 729 | 588 | 365 | 865 |
| 136 | 636 | −050 | 996 | −224 | −934 | 482 | 802 | −703 | −608 | 870 | 368 | 364 | 864 |
| 137 | 637 | 088 | 972 | −380 | −858 | 637 | 666 | −838 | −414 | 962 | 125 | 363 | 863 |
| 138 | 638 | 224 | 925 | −525 | −754 | 771 | 504 | −934 | −200 | 999 | −125 | 362 | 862 |
| 139 | 639 | 356 | 858 | −657 | −628 | 876 | 321 | −989 | 025 | 980 | −368 | 361 | 861 |
| | | | | | | | | | | | | | |
| 140 | 640 | 482 | 771 | −771 | −482 | 951 | 125 | −998 | 249 | 905 | −588 | 360 | 860 |
| 141 | 641 | 598 | 666 | −864 | −321 | 992 | −075 | −962 | 460 | 778 | −771 | 359 | 859 |
| 142 | 642 | 703 | 546 | −934 | −150 | 998 | −273 | −882 | 647 | 608 | −905 | 358 | 858 |
| 143 | 643 | 794 | 414 | −980 | 025 | 969 | −460 | −762 | 802 | 403 | −982 | 357 | 857 |
| 144 | 644 | 870 | 273 | −999 | 200 | 905 | −628 | −608 | 915 | 175 | −998 | 356 | 856 |
| | | | | | | | | | | | | | |
| 145 | 645 | 930 | 125 | −992 | 368 | 809 | −771 | −426 | 982 | −063 | −951 | 355 | 855 |
| 146 | 646 | 972 | −025 | −959 | 525 | 685 | −882 | −224 | 999 | −297 | −844 | 354 | 954 |
| 147 | 647 | 995 | −175 | −899 | 666 | 536 | −959 | −013 | 965 | −514 | −685 | 353 | 853 |
| 148 | 648 | 999 | −321 | −816 | 786 | 368 | −996 | 200 | 882 | −703 | −482 | 352 | 852 |
| 149 | 649 | 985 | −460 | −712 | 882 | 187 | −994 | 403 | 754 | −851 | −249 | 351 | 851 |
| | | | | | | | | | | | | | |
| 150 | 650 | 951 | −588 | −588 | 951 | 000 | −951 | 588 | 588 | −951 | 000 | 350 | 850 |
| 151 | 651 | 899 | −703 | −448 | 990 | −187 | −870 | 746 | 391 | −997 | 249 | 349 | 849 |
| 152 | 652 | 831 | −802 | −297 | 999 | −368 | −754 | 870 | 175 | −987 | 482 | 348 | 848 |
| 153 | 653 | 746 | −882 | −138 | 977 | −536 | −608 | 955 | −050 | −920 | 685 | 347 | 847 |
| 154 | 654 | 647 | −943 | 025 | 925 | −685 | −437 | 996 | −273 | −802 | 844 | 346 | 846 |
| | | | | | | | | | | | | | |
| 155 | 655 | 536 | −982 | 187 | 844 | −809 | −249 | 992 | −482 | −637 | 951 | 345 | 845 |
| 156 | 656 | 414 | −999 | 345 | 738 | −905 | −050 | 943 | −666 | −437 | 998 | 344 | 844 |
| 157 | 657 | 285 | −994 | 493 | 608 | −969 | 150 | 851 | −816 | −212 | 982 | 343 | 843 |
| 158 | 658 | 150 | −965 | 628 | 460 | −998 | 345 | 720 | −925 | 025 | 905 | 342 | 842 |
| 159 | 659 | 013 | −915 | 746 | 297 | −992 | 525 | 557 | −987 | 261 | 771 | 341 | 841 |
| | | | | | | | | | | | | | |
| 160 | 660 | −125 | −844 | 844 | 125 | −951 | 685 | 368 | −998 | 482 | 588 | 340 | 840 |
| 161 | 661 | −261 | −754 | 920 | −050 | −876 | 816 | 163 | −959 | 675 | 368 | 339 | 839 |
| 162 | 662 | −391 | −647 | 972 | −224 | −771 | 915 | −050 | −870 | 831 | 125 | 338 | 838 |
| 163 | 663 | −514 | −525 | 997 | −391 | −637 | 977 | −261 | −738 | 939 | −125 | 337 | 837 |
| 164 | 664 | −628 | −391 | 996 | −546 | −482 | 1000 | −460 | −567 | 994 | −368 | 336 | 836 |
| | | | | | | | | | | | | | |
| 165 | 665 | −729 | −249 | 969 | −685 | −309 | 982 | −637 | −368 | 992 | −588 | 335 | 835 |
| 166 | 666 | −816 | −100 | 915 | −802 | −125 | 925 | −786 | −150 | 934 | −771 | 334 | 834 |
| 167 | 667 | −888 | 050 | 838 | −894 | 063 | 831 | −899 | 075 | 824 | −905 | 333 | 833 |
| 168 | 668 | −943 | 200 | 738 | −959 | 249 | 703 | −972 | 297 | 666 | −982 | 332 | 832 |
| 169 | 669 | −980 | 345 | 618 | −994 | 426 | 546 | −1000 | 504 | 471 | −998 | 331 | 831 |
| | | | | | | | | | | | | | |
| 170 | 670 | −998 | 482 | 482 | −998 | 588 | 368 | −982 | 685 | 249 | −951 | 330 | 830 |
| 171 | 671 | −997 | 608 | 333 | −972 | 729 | 175 | −920 | 831 | 013 | −844 | 329 | 829 |
| 172 | 672 | −977 | 720 | 175 | −915 | 844 | −025 | −816 | 934 | −224 | −685 | 328 | 828 |
| 173 | 673 | −939 | 816 | 013 | −831 | 930 | −224 | −675 | 990 | −448 | −482 | 327 | 827 |
| 174 | 674 | −882 | 894 | −150 | −720 | 982 | −414 | −504 | 996 | −647 | −249 | 326 | 826 |
| | | | | | | | | | | | | | |
| 175 | 675 | −809 | 951 | −309 | −588 | 1000 | −588 | −309 | 951 | −809 | 000 | 325 | 825 |
| 176 | 676 | −720 | 987 | −460 | −437 | 982 | −738 | −100 | 858 | −925 | 249 | 324 | 824 |
| 177 | 677 | −618 | 1000 | −598 | −273 | 930 | −858 | 113 | 720 | −989 | 482 | 323 | 823 |
| 178 | 678 | −504 | 990 | −720 | −100 | 844 | −943 | 321 | 546 | −996 | 685 | 322 | 822 |
| 179 | 679 | −380 | 959 | −824 | 075 | 729 | −990 | 514 | 345 | −947 | 844 | 321 | 821 |

TABLE 8.5B (*continued*)
 $\sin 2\pi hx$ (h even) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=2$ | 4 | 6 | 8 | 10 | 12 | 14 | 16 | 18 | 20 | Change sign.
x | |
|-----------------------|-----|-------|-------|------|-------|------|------|------|------|------|------|---------------------|-----|
| 180 | 680 | 771 | −982 | 482 | 368 | −951 | 844 | −125 | −685 | 998 | −588 | 320 | 820 |
| 181 | 681 | 762 | −987 | 514 | 321 | −930 | 882 | −212 | −608 | 999 | −685 | 319 | 819 |
| 182 | 682 | 754 | −990 | 546 | 273 | −905 | 915 | −297 | −525 | 987 | −771 | 318 | 818 |
| 183 | 683 | 746 | −994 | 578 | 224 | −876 | 943 | −380 | −437 | 962 | −844 | 317 | 817 |
| 184 | 684 | 738 | −996 | 608 | 175 | −844 | 965 | −460 | −345 | 925 | −905 | 316 | 816 |
| | | | | | | | | | | | | | |
| 185 | 685 | 729 | −998 | 637 | 125 | −809 | 982 | −536 | −249 | 876 | −951 | 315 | 815 |
| 186 | 686 | 720 | −999 | 666 | 075 | −771 | 994 | −608 | −150 | 816 | −982 | 314 | 814 |
| 187 | 687 | 712 | −1000 | 694 | 025 | −729 | 999 | −675 | −050 | 746 | −998 | 313 | 813 |
| 188 | 688 | 703 | −1000 | 720 | −025 | −685 | 999 | −738 | 050 | 666 | −998 | 312 | 812 |
| 189 | 689 | 694 | −999 | 746 | −075 | −637 | 994 | −794 | 150 | 578 | −982 | 311 | 811 |
| | | | | | | | | | | | | | |
| 190 | 690 | 685 | −998 | 771 | −125 | −588 | 982 | −844 | 249 | 482 | −951 | 310 | 810 |
| 191 | 691 | 675 | −996 | 794 | −175 | −536 | 965 | −888 | 345 | 380 | −905 | 309 | 809 |
| 192 | 692 | 666 | −994 | 816 | −224 | −482 | 943 | −925 | 437 | 273 | −844 | 308 | 808 |
| 193 | 693 | 657 | −990 | 838 | −273 | −426 | 915 | −955 | 525 | 163 | −771 | 307 | 807 |
| 194 | 694 | 647 | −987 | 858 | −321 | −368 | 882 | −977 | 608 | 050 | −685 | 306 | 806 |
| | | | | | | | | | | | | | |
| 195 | 695 | 637 | −982 | 876 | −368 | −309 | 844 | −992 | 685 | −063 | −588 | 305 | 805 |
| 196 | 696 | 628 | −977 | 894 | −414 | −249 | 802 | −999 | 754 | −175 | −482 | 304 | 804 |
| 197 | 697 | 618 | −972 | 910 | −460 | −187 | 754 | −999 | 816 | −285 | −368 | 303 | 803 |
| 198 | 698 | 608 | −965 | 925 | −504 | −125 | 703 | −990 | 870 | −391 | −249 | 302 | 802 |
| 199 | 699 | 598 | −959 | 939 | −546 | −063 | 647 | −975 | 915 | −493 | −125 | 301 | 801 |
| | | | | | | | | | | | | | |
| 200 | 700 | 588 | −951 | 951 | −588 | 000 | 588 | −951 | 951 | −588 | 000 | 300 | 800 |
| 201 | 701 | 578 | −943 | 962 | −628 | 063 | 525 | −920 | 977 | −675 | 125 | 299 | 799 |
| 202 | 702 | 567 | −934 | 972 | −666 | 125 | 460 | −882 | 994 | −754 | 249 | 298 | 798 |
| 203 | 703 | 557 | −925 | 980 | −703 | 187 | 391 | −838 | 1000 | −824 | 368 | 297 | 797 |
| 204 | 704 | 546 | −915 | 987 | −738 | 249 | 321 | −786 | 996 | −882 | 482 | 296 | 796 |
| | | | | | | | | | | | | | |
| 205 | 705 | 536 | −905 | 992 | −771 | 309 | 249 | −729 | 982 | −930 | 588 | 295 | 795 |
| 206 | 706 | 525 | −894 | 996 | −802 | 368 | 175 | −666 | 959 | −965 | 685 | 294 | 794 |
| 207 | 707 | 514 | −882 | 999 | −831 | 426 | 100 | −598 | 925 | −989 | 771 | 293 | 793 |
| 208 | 708 | 504 | −870 | 1000 | −858 | 482 | 025 | −525 | 882 | −999 | 844 | 292 | 792 |
| 209 | 709 | 493 | −858 | 1000 | −882 | 536 | −050 | −448 | 831 | −997 | 905 | 291 | 791 |
| | | | | | | | | | | | | | |
| 210 | 710 | 482 | −844 | 998 | −905 | 588 | −125 | −368 | 771 | −982 | 951 | 290 | 790 |
| 211 | 711 | 471 | −831 | 995 | −925 | 637 | −200 | −285 | 703 | −955 | 982 | 289 | 789 |
| 212 | 712 | 460 | −816 | 990 | −943 | 685 | −273 | −200 | 628 | −915 | 998 | 288 | 788 |
| 213 | 713 | 448 | −802 | 985 | −959 | 729 | −345 | −113 | 546 | −864 | 998 | 287 | 787 |
| 214 | 714 | 437 | −786 | 977 | −972 | 771 | −414 | −025 | 460 | −802 | 982 | 286 | 786 |
| | | | | | | | | | | | | | |
| 215 | 715 | 426 | −771 | 969 | −982 | 809 | −482 | 063 | 368 | −729 | 951 | 285 | 785 |
| 216 | 716 | 414 | −754 | 959 | −990 | 844 | −546 | 150 | 273 | −647 | 905 | 284 | 784 |
| 217 | 717 | 403 | −738 | 947 | −996 | 876 | −608 | 237 | 175 | −557 | 844 | 283 | 783 |
| 218 | 718 | 391 | −720 | 934 | −999 | 905 | −666 | 321 | 075 | −460 | 771 | 282 | 782 |
| 219 | 719 | 380 | −703 | 920 | −1000 | 930 | −720 | 403 | −025 | −356 | 685 | 281 | 781 |
| | | | | | | | | | | | | | |
| 220 | 720 | 368 | −685 | 905 | −998 | 951 | −771 | 482 | −125 | −249 | 588 | 280 | 780 |
| 221 | 721 | 356 | −666 | 888 | −994 | 969 | −816 | 557 | −224 | −138 | 482 | 279 | 779 |
| 222 | 722 | 345 | −647 | 870 | −987 | 982 | −858 | 628 | −321 | −025 | 368 | 278 | 778 |
| 223 | 723 | 333 | −628 | 851 | −977 | 992 | −894 | 694 | −414 | 088 | 249 | 277 | 777 |
| 224 | 724 | 321 | −608 | 831 | −965 | 998 | −925 | 754 | −504 | 200 | 125 | 276 | 776 |

TABLE 8.5B (continued)

$\sin 2\pi hx$ (h even) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=22$ | 24 | 26 | 28 | 30 | 32 | 34 | 36 | 38 | 40 | Change sign.
x | |
|-----------------------|-----|--------|-------|-------|------|------|-------|------|------|-------|------|---------------------|-----|
| 180 | 680 | −249 | 905 | −905 | 249 | 588 | −998 | 685 | 125 | −844 | 951 | 320 | 820 |
| 181 | 681 | −113 | 831 | −962 | 414 | 426 | −965 | 824 | −100 | −694 | 998 | 319 | 819 |
| 182 | 682 | 025 | 738 | −994 | 567 | 249 | −894 | 925 | −321 | −504 | 982 | 318 | 818 |
| 183 | 683 | 163 | 628 | −999 | 703 | 063 | −786 | 985 | −525 | −285 | 905 | 317 | 817 |
| 184 | 684 | 297 | 504 | −977 | 816 | −125 | −647 | 999 | −703 | −050 | 771 | 316 | 816 |
| 185 | 685 | 426 | 368 | −930 | 905 | −309 | −482 | 969 | −844 | 187 | 588 | 315 | 815 |
| 186 | 686 | 546 | 224 | −858 | 965 | −482 | −297 | 894 | −943 | 414 | 368 | 314 | 814 |
| 187 | 687 | 657 | 075 | −762 | 996 | −637 | −100 | 778 | −994 | 618 | 125 | 313 | 813 |
| 188 | 688 | 754 | −075 | −647 | 996 | −771 | 100 | 628 | −994 | 786 | −125 | 312 | 812 |
| 189 | 689 | 838 | −224 | −514 | 965 | −876 | 297 | 448 | −943 | 910 | −368 | 311 | 811 |
| 190 | 690 | 905 | −368 | −368 | 905 | −951 | 482 | 249 | −844 | 982 | −588 | 310 | 810 |
| 191 | 691 | 955 | −504 | −212 | 816 | −992 | 647 | 038 | −703 | 999 | −771 | 309 | 809 |
| 192 | 692 | 987 | −628 | −050 | 703 | −998 | 786 | −175 | −525 | 959 | −905 | 308 | 808 |
| 193 | 693 | 1000 | −738 | 113 | 567 | −969 | 894 | −380 | −321 | 864 | −982 | 307 | 807 |
| 194 | 694 | 994 | −831 | 273 | 414 | −905 | 965 | −567 | −100 | 720 | −998 | 306 | 806 |
| 195 | 695 | 969 | −905 | 426 | 249 | −809 | 998 | −729 | 125 | 536 | −951 | 305 | 805 |
| 196 | 696 | 925 | −959 | 567 | 075 | −685 | 990 | −858 | 345 | 321 | −844 | 304 | 804 |
| 197 | 697 | 864 | −990 | 694 | −100 | −536 | 943 | −947 | 546 | 088 | −685 | 303 | 803 |
| 198 | 698 | 786 | −1000 | 802 | −273 | −368 | 858 | −994 | 720 | −150 | −482 | 302 | 802 |
| 199 | 699 | 694 | −987 | 888 | −437 | −187 | 738 | −995 | 858 | −380 | −249 | 301 | 801 |
| 200 | 700 | 588 | −951 | 951 | −588 | 000 | 588 | −951 | 951 | −588 | 000 | 300 | 800 |
| 201 | 701 | 471 | −894 | 989 | −720 | 187 | 414 | −864 | 996 | −762 | 249 | 299 | 799 |
| 202 | 702 | 345 | −816 | 1000 | −831 | 368 | 224 | −738 | 990 | −894 | 482 | 298 | 798 |
| 203 | 703 | 212 | −720 | 985 | −915 | 536 | 025 | −578 | 934 | −975 | 685 | 297 | 797 |
| 204 | 704 | 075 | −608 | 943 | −972 | 685 | −175 | −391 | 831 | −1000 | 844 | 296 | 796 |
| 205 | 705 | −063 | −482 | 876 | −998 | 809 | −368 | −187 | 685 | −969 | 951 | 295 | 795 |
| 206 | 706 | −200 | −345 | 786 | −994 | 905 | −546 | 025 | 504 | −882 | 998 | 294 | 794 |
| 207 | 707 | −333 | −200 | 675 | −959 | 969 | −703 | 237 | 297 | −746 | 982 | 293 | 793 |
| 208 | 708 | −460 | −050 | 546 | −894 | 998 | −831 | 437 | 075 | −567 | 905 | 292 | 792 |
| 209 | 709 | −578 | 100 | 403 | −802 | 992 | −925 | 618 | −150 | −356 | 771 | 291 | 791 |
| 210 | 710 | −685 | 249 | 249 | −685 | 951 | −982 | 771 | −368 | −125 | 588 | 290 | 790 |
| 211 | 711 | −778 | 391 | 088 | −546 | 876 | −1000 | 888 | −567 | 113 | 368 | 289 | 789 |
| 212 | 712 | −858 | 525 | −075 | −391 | 771 | −977 | 965 | −738 | 345 | 125 | 288 | 788 |
| 213 | 713 | −920 | 647 | −237 | −224 | 637 | −915 | 999 | −870 | 557 | −125 | 287 | 787 |
| 214 | 714 | −965 | 754 | −391 | −050 | 482 | −816 | 987 | −959 | 738 | −368 | 286 | 786 |
| 215 | 715 | −992 | 844 | −536 | 125 | 309 | −685 | 930 | −998 | 876 | −588 | 285 | 785 |
| 216 | 716 | −1000 | 915 | −666 | 297 | 125 | −525 | 831 | −987 | 965 | −771 | 284 | 784 |
| 217 | 717 | −989 | 965 | −778 | 460 | −063 | −345 | 694 | −925 | 1000 | −905 | 283 | 783 |
| 218 | 718 | −959 | 994 | −870 | 608 | −249 | −150 | 525 | −816 | 977 | −982 | 282 | 782 |
| 219 | 719 | −910 | 999 | −939 | 738 | −426 | 050 | 333 | −666 | 899 | −998 | 281 | 781 |
| 220 | 720 | −844 | 982 | −982 | 844 | −588 | 249 | 125 | −482 | 771 | −951 | 280 | 780 |
| 221 | 721 | −762 | 943 | −1000 | 925 | −729 | 437 | −088 | −273 | 598 | −844 | 279 | 779 |
| 222 | 722 | −666 | 882 | −990 | 977 | −844 | 608 | −297 | −050 | 391 | −685 | 278 | 778 |
| 223 | 723 | −557 | 802 | −955 | 999 | −930 | 754 | −493 | 175 | 163 | −482 | 277 | 777 |
| 224 | 724 | −437 | 703 | −894 | 990 | −982 | 870 | −666 | 391 | −075 | −249 | 276 | 776 |

TABLE 8.5B (continued)

 $\sin 2\pi hx$ (h even) (x fractional. Decimal points omitted throughout)

| Sign as given..
x | | $h=2$ | 4 | 6 | 8 | 10 | 12 | 14 | 16 | 18 | 20 | Change sign..
x | |
|------------------------|-----|-------|------|-----|------|------|-------|------|------|------|------|----------------------|-----|
| 225 | 725 | 309 | -588 | 809 | -951 | 1000 | -951 | 809 | -588 | 309 | 000 | 275 | 775 |
| 226 | 726 | 297 | -567 | 786 | -934 | 998 | -972 | 858 | -666 | 414 | -125 | 274 | 774 |
| 227 | 727 | 285 | -546 | 762 | -915 | 992 | -987 | 899 | -738 | 514 | -249 | 273 | 773 |
| 228 | 728 | 273 | -525 | 738 | -894 | 982 | -996 | 934 | -802 | 608 | -368 | 272 | 772 |
| 229 | 729 | 261 | -504 | 712 | -870 | 969 | -1000 | 962 | -858 | 694 | -482 | 271 | 771 |
| | | | | | | | | | | | | | |
| 230 | 730 | 249 | -482 | 685 | -844 | 951 | -998 | 982 | -905 | 771 | -588 | 270 | 770 |
| 231 | 731 | 237 | -460 | 657 | -816 | 930 | -990 | 995 | -943 | 838 | -685 | 269 | 769 |
| 232 | 732 | 224 | -437 | 628 | -786 | 905 | -977 | 1000 | -972 | 894 | -771 | 268 | 768 |
| 233 | 733 | 212 | -414 | 598 | -754 | 876 | -959 | 997 | -990 | 939 | -844 | 267 | 767 |
| 234 | 734 | 200 | -391 | 567 | -720 | 844 | -934 | 987 | -999 | 972 | -905 | 266 | 766 |
| | | | | | | | | | | | | | |
| 235 | 735 | 187 | -368 | 536 | -685 | 809 | -905 | 969 | -998 | 992 | -951 | 265 | 765 |
| 236 | 736 | 175 | -345 | 504 | -647 | 771 | -870 | 943 | -987 | 1000 | -982 | 264 | 764 |
| 237 | 737 | 163 | -321 | 471 | -608 | 729 | -831 | 910 | -965 | 995 | -998 | 263 | 763 |
| 238 | 738 | 150 | -297 | 437 | -567 | 685 | -786 | 870 | -934 | 977 | -998 | 262 | 762 |
| 239 | 739 | 138 | -273 | 403 | -525 | 637 | -738 | 824 | -894 | 947 | -982 | 261 | 761 |
| | | | | | | | | | | | | | |
| 240 | 740 | 125 | -249 | 368 | -482 | 588 | -685 | 771 | -844 | 905 | -951 | 260 | 760 |
| 241 | 741 | 113 | -224 | 333 | -437 | 536 | -628 | 712 | -786 | 851 | -905 | 259 | 759 |
| 242 | 742 | 100 | -200 | 297 | -391 | 482 | -567 | 647 | -720 | 786 | -844 | 258 | 758 |
| 243 | 743 | 088 | -175 | 261 | -345 | 426 | -504 | 578 | -647 | 712 | -771 | 257 | 757 |
| 244 | 744 | 075 | -150 | 224 | -297 | 368 | -437 | 504 | -567 | 628 | -685 | 256 | 756 |
| | | | | | | | | | | | | | |
| 245 | 745 | 063 | -125 | 187 | -249 | 309 | -368 | 426 | -482 | 536 | -588 | 255 | 755 |
| 246 | 746 | 050 | -100 | 150 | -200 | 249 | -297 | 345 | -391 | 437 | -482 | 254 | 754 |
| 247 | 747 | 038 | -075 | 113 | -150 | 187 | -224 | 261 | -297 | 333 | -368 | 253 | 753 |
| 248 | 748 | 025 | -050 | 075 | -100 | 125 | -150 | 176 | -200 | 224 | -249 | 252 | 752 |
| 249 | 749 | 013 | -025 | 038 | -050 | 063 | -075 | 088 | -100 | 113 | -125 | 251 | 751 |
| | | | | | | | | | | | | | |
| 250 | 750 | 000 | 000 | 000 | 000 | 000 | 000 | 000 | 000 | 000 | 000 | 250 | 750 |

TABLE 8.5B (*continued*)
 $\sin 2\pi hx$ (h even) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=22$ | 24 | 26 | 28 | 30 | 32 | 34 | 36 | 38 | 40 | Change sign.
x | |
|-----------------------|-----|--------|------|------|-------|-------|------|-------|-------|------|------|---------------------|-----|
| 225 | 725 | −309 | 588 | −809 | 951 | −1000 | 951 | −809 | 588 | −309 | 000 | 275 | 775 |
| 226 | 726 | −175 | 460 | −703 | 882 | −982 | 994 | −915 | 754 | −525 | 249 | 274 | 774 |
| 227 | 727 | −038 | 321 | −578 | 786 | −930 | 996 | −980 | 882 | −712 | 482 | 273 | 773 |
| 228 | 728 | 100 | 175 | −437 | 666 | −844 | 959 | −1000 | 965 | −858 | 685 | 272 | 772 |
| 229 | 729 | 237 | 025 | −285 | 525 | −729 | 882 | −975 | 999 | −955 | 844 | 271 | 771 |
| | | | | | | | | | | | | | |
| 230 | 730 | 368 | −125 | −125 | 368 | −588 | 771 | −905 | 982 | −998 | 951 | 270 | 770 |
| 231 | 731 | 493 | −273 | 038 | 200 | −426 | 628 | −794 | 915 | −985 | 998 | 269 | 769 |
| 232 | 732 | 608 | −414 | 200 | 025 | −249 | 460 | −647 | 802 | −915 | 982 | 268 | 768 |
| 233 | 733 | 712 | −546 | 356 | −150 | −063 | 273 | −471 | 647 | −794 | 905 | 267 | 767 |
| 234 | 734 | 802 | −666 | 504 | −321 | 125 | 075 | −273 | 460 | −628 | 771 | 266 | 766 |
| | | | | | | | | | | | | | |
| 235 | 735 | 876 | −771 | 637 | −482 | 309 | −125 | −063 | 249 | −426 | 588 | 265 | 765 |
| 236 | 736 | 934 | −858 | 754 | −628 | 482 | −321 | 150 | 025 | −200 | 368 | 264 | 764 |
| 237 | 737 | 975 | −925 | 851 | −754 | 637 | −504 | 356 | −200 | 038 | 125 | 263 | 763 |
| 238 | 738 | 996 | −972 | 925 | −858 | 771 | −666 | 546 | −414 | 273 | −125 | 262 | 762 |
| 239 | 739 | 999 | −996 | 975 | −934 | 876 | −802 | 712 | −608 | 493 | −368 | 261 | 761 |
| | | | | | | | | | | | | | |
| 240 | 740 | 982 | −998 | 998 | −982 | 951 | −905 | 844 | −771 | 685 | −588 | 260 | 760 |
| 241 | 741 | 947 | −977 | 995 | −1000 | 992 | −972 | 939 | −894 | 838 | −771 | 259 | 759 |
| 242 | 742 | 894 | −934 | 965 | −987 | 998 | −999 | 990 | −972 | 943 | −905 | 258 | 758 |
| 243 | 743 | 824 | −870 | 910 | −943 | 969 | −987 | 997 | −1000 | 995 | −982 | 257 | 757 |
| 244 | 744 | 738 | −786 | 831 | −870 | 905 | −934 | 959 | −977 | 990 | −998 | 256 | 756 |
| | | | | | | | | | | | | | |
| 245 | 745 | 637 | −685 | 729 | −771 | 809 | −844 | 876 | −905 | 930 | −951 | 255 | 755 |
| 246 | 746 | 525 | −567 | 608 | −647 | 685 | −720 | 754 | −786 | 816 | −844 | 254 | 754 |
| 247 | 747 | 403 | −437 | 471 | −504 | 536 | −567 | 598 | −628 | 657 | −685 | 253 | 753 |
| 248 | 748 | 273 | −297 | 321 | −345 | 368 | −391 | 414 | −437 | 460 | −482 | 252 | 752 |
| 249 | 749 | 138 | −150 | 163 | −175 | 187 | −200 | 212 | −224 | 237 | −249 | 251 | 751 |
| | | | | | | | | | | | | | |
| 250 | 750 | 000 | 000 | 000 | 000 | 000 | 000 | 000 | 000 | 000 | 000 | 250 | 750 |

TABLE 8.5C
 $\cos 2\pi hx$ (h odd) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=1$ | 3 | 5 | 7 | 9 | 11 | 13 | 15 | 17 | 19 | Change sign.
x | |
|-----------------------|------|-------|------|------|------|------|------|------|-------|------|------|---------------------|-----|
| 000 | 1000 | 1000 | 1000 | 1000 | 1000 | 1000 | 1000 | 1000 | 1000 | 1000 | 1000 | 500 | 500 |
| 001 | 999 | 1000 | 1000 | 1000 | 999 | 998 | 998 | 997 | 996 | 994 | 993 | 499 | 501 |
| 002 | 998 | 1000 | 999 | 998 | 996 | 994 | 990 | 987 | 982 | 977 | 972 | 498 | 502 |
| 003 | 997 | 1000 | 998 | 996 | 991 | 986 | 979 | 970 | 960 | 949 | 937 | 497 | 503 |
| 004 | 996 | 1000 | 997 | 992 | 985 | 975 | 962 | 947 | 930 | 910 | 888 | 496 | 504 |
| | | | | | | | | | | | | | |
| 005 | 995 | 1000 | 996 | 988 | 976 | 960 | 941 | 918 | 891 | 861 | 827 | 495 | 505 |
| 006 | 994 | 999 | 994 | 982 | 965 | 943 | 915 | 882 | 844 | 802 | 754 | 494 | 506 |
| 007 | 993 | 999 | 991 | 976 | 953 | 923 | 885 | 841 | 790 | 733 | 671 | 493 | 507 |
| 008 | 992 | 999 | 989 | 969 | 939 | 899 | 851 | 794 | 729 | 657 | 578 | 492 | 508 |
| 009 | 991 | 998 | 986 | 960 | 923 | 873 | 813 | 742 | 661 | 572 | 476 | 491 | 509 |
| | | | | | | | | | | | | | |
| 010 | 990 | 998 | 982 | 951 | 905 | 844 | 771 | 685 | 588 | 482 | 368 | 490 | 510 |
| 011 | 989 | 998 | 979 | 941 | 885 | 813 | 725 | 623 | 509 | 386 | 255 | 489 | 511 |
| 012 | 988 | 997 | 975 | 930 | 864 | 778 | 675 | 557 | 426 | 285 | 138 | 488 | 512 |
| 013 | 987 | 997 | 970 | 918 | 841 | 742 | 623 | 487 | 339 | 181 | 019 | 487 | 513 |
| 014 | 986 | 996 | 965 | 905 | 816 | 703 | 567 | 414 | 249 | 075 | -100 | 486 | 514 |
| | | | | | | | | | | | | | |
| 015 | 985 | 996 | 960 | 891 | 790 | 661 | 509 | 339 | 156 | -031 | -218 | 485 | 515 |
| 016 | 984 | 995 | 955 | 876 | 762 | 618 | 448 | 261 | 063 | -138 | -333 | 484 | 516 |
| 017 | 983 | 994 | 949 | 861 | 733 | 572 | 386 | 181 | -031 | -243 | -443 | 483 | 517 |
| 018 | 982 | 994 | 943 | 844 | 703 | 525 | 321 | 100 | -125 | -345 | -546 | 482 | 518 |
| 019 | 981 | 993 | 937 | 827 | 671 | 476 | 255 | 019 | -218 | -443 | -642 | 481 | 519 |
| | | | | | | | | | | | | | |
| 020 | 980 | 992 | 930 | 809 | 637 | 426 | 187 | -063 | -309 | -536 | -729 | 480 | 520 |
| 021 | 979 | 991 | 923 | 790 | 603 | 374 | 119 | -144 | -397 | -623 | -805 | 479 | 521 |
| 022 | 978 | 990 | 915 | 771 | 567 | 321 | 050 | -224 | -482 | -703 | -870 | 478 | 522 |
| 023 | 977 | 990 | 907 | 750 | 531 | 267 | -019 | -303 | -562 | -775 | -923 | 477 | 523 |
| 024 | 976 | 989 | 899 | 729 | 493 | 212 | -088 | -380 | -637 | -838 | -962 | 476 | 524 |
| | | | | | | | | | | | | | |
| 025 | 975 | 988 | 891 | 707 | 454 | 156 | -156 | -454 | -707 | -891 | -988 | 475 | 525 |
| 026 | 974 | 987 | 882 | 685 | 414 | 100 | -224 | -525 | -771 | -934 | -999 | 474 | 526 |
| 027 | 973 | 986 | 873 | 661 | 374 | 044 | -291 | -593 | -827 | -967 | -997 | 473 | 527 |
| 028 | 972 | 985 | 864 | 637 | 333 | -013 | -356 | -657 | -876 | -989 | -980 | 472 | 528 |
| 029 | 971 | 983 | 854 | 613 | 291 | -069 | -420 | -716 | -918 | -999 | -949 | 471 | 529 |
| | | | | | | | | | | | | | |
| 030 | 970 | 982 | 844 | 588 | 249 | -125 | -482 | -771 | -951 | -998 | -905 | 470 | 530 |
| 031 | 969 | 981 | 834 | 562 | 206 | -181 | -541 | -820 | -976 | -986 | -848 | 469 | 531 |
| 032 | 968 | 980 | 824 | 536 | 163 | -237 | -598 | -864 | -992 | -962 | -778 | 468 | 532 |
| 033 | 967 | 979 | 813 | 509 | 119 | -291 | -652 | -902 | -1000 | -927 | -698 | 467 | 533 |
| 034 | 966 | 977 | 802 | 482 | 075 | -345 | -703 | -934 | -998 | -882 | -608 | 466 | 534 |
| | | | | | | | | | | | | | |
| 035 | 965 | 976 | 790 | 454 | 031 | -397 | -750 | -960 | -988 | -827 | -509 | 465 | 535 |
| 036 | 964 | 975 | 778 | 426 | -013 | -448 | -794 | -980 | -969 | -762 | -403 | 464 | 536 |
| 037 | 963 | 973 | 767 | 397 | -057 | -498 | -834 | -993 | -941 | -689 | -291 | 463 | 537 |
| 038 | 962 | 972 | 754 | 368 | -100 | -546 | -870 | -999 | -905 | -608 | -175 | 462 | 538 |
| 039 | 961 | 970 | 742 | 339 | -144 | -593 | -902 | -999 | -861 | -520 | -057 | 461 | 539 |
| | | | | | | | | | | | | | |
| 040 | 960 | 969 | 729 | 309 | -187 | -637 | -930 | -992 | -809 | -426 | 063 | 460 | 540 |
| 041 | 959 | 967 | 716 | 279 | -230 | -680 | -953 | -979 | -750 | -327 | 181 | 459 | 541 |
| 042 | 958 | 965 | 703 | 249 | -273 | -720 | -972 | -959 | -685 | -224 | 297 | 458 | 542 |
| 043 | 957 | 964 | 689 | 218 | -315 | -758 | -986 | -932 | -613 | -119 | 409 | 457 | 543 |
| 044 | 956 | 962 | 675 | 187 | -356 | -794 | -995 | -899 | -536 | -013 | 514 | 456 | 544 |

TABLE 8.5C

 $\cos 2\pi hx$ (h odd) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=21$ | 23 | 25 | 27 | 29 | 31 | 33 | 35 | 37 | 39 | Change sign.
x | |
|-----------------------|------|--------|------|-------|------|------|-------|-------|-------|------|------|---------------------|-----|
| 000 | 1000 | 1000 | 1000 | 1000 | 1000 | 1000 | 1000 | 1000 | 1000 | 1000 | 1000 | 500 | 500 |
| 001 | 999 | 991 | 990 | 988 | 986 | 983 | 981 | 979 | 976 | 973 | 970 | 499 | 501 |
| 002 | 998 | 965 | 959 | 951 | 943 | 934 | 925 | 915 | 905 | 894 | 882 | 498 | 502 |
| 003 | 997 | 923 | 907 | 891 | 873 | 854 | 834 | 813 | 790 | 767 | 742 | 497 | 503 |
| 004 | 996 | 864 | 838 | 809 | 778 | 746 | 712 | 675 | 637 | 598 | 557 | 496 | 504 |
| | | | | | | | | | | | | | |
| 005 | 995 | 790 | 750 | 707 | 661 | 613 | 562 | 509 | 454 | 397 | 339 | 495 | 505 |
| 006 | 994 | 703 | 647 | 588 | 525 | 460 | 391 | 321 | 249 | 175 | 100 | 494 | 506 |
| 007 | 993 | 603 | 531 | 454 | 374 | 291 | 206 | 119 | 031 | -057 | -144 | 493 | 507 |
| 008 | 992 | 493 | 403 | 309 | 212 | 113 | 013 | -088 | -187 | -285 | -380 | 492 | 508 |
| 009 | 991 | 374 | 267 | 156 | 044 | -069 | -181 | -291 | -397 | -498 | -593 | 491 | 509 |
| | | | | | | | | | | | | | |
| 010 | 990 | 249 | 125 | 000 | -125 | -249 | -368 | -482 | -588 | -685 | -771 | 490 | 510 |
| 011 | 989 | 119 | -019 | -156 | -291 | -420 | -541 | -652 | -750 | -834 | -902 | 489 | 511 |
| 012 | 988 | -013 | -163 | -309 | -448 | -578 | -694 | -794 | -876 | -939 | -980 | 488 | 512 |
| 013 | 987 | -144 | -303 | -454 | -593 | -716 | -820 | -902 | -960 | -993 | -999 | 487 | 513 |
| 014 | 986 | -273 | -437 | -588 | -720 | -831 | -915 | -972 | -998 | -994 | -959 | 486 | 514 |
| | | | | | | | | | | | | | |
| 015 | 985 | -397 | -562 | -707 | -827 | -918 | -976 | -1000 | -988 | -941 | -861 | 485 | 515 |
| 016 | 984 | -514 | -675 | -809 | -910 | -975 | -1000 | -985 | -930 | -838 | -712 | 484 | 516 |
| 017 | 983 | -623 | -775 | -891 | -967 | -999 | -986 | -927 | -827 | -689 | -520 | 483 | 517 |
| 018 | 982 | -720 | -858 | -951 | -996 | -990 | -934 | -831 | -685 | -504 | -297 | 482 | 518 |
| 019 | 981 | -805 | -923 | -988 | -997 | -949 | -848 | -698 | -509 | -291 | -057 | 481 | 519 |
| | | | | | | | | | | | | | |
| 020 | 980 | -876 | -969 | -1000 | -969 | -876 | -729 | -536 | -309 | -063 | 187 | 480 | 520 |
| 021 | 979 | -932 | -994 | -988 | -913 | -775 | -583 | -351 | -094 | 169 | 420 | 479 | 521 |
| 022 | 978 | -972 | -999 | -951 | -831 | -647 | -414 | -150 | 125 | 391 | 628 | 478 | 522 |
| 023 | 977 | -994 | -983 | -891 | -725 | -498 | -230 | 057 | 339 | 593 | 798 | 477 | 523 |
| 024 | 976 | -1000 | -947 | -809 | -598 | -333 | -038 | 261 | 536 | 762 | 920 | 476 | 524 |
| | | | | | | | | | | | | | |
| 025 | 975 | -988 | -891 | -707 | -454 | -156 | 156 | 454 | 707 | 891 | 988 | 475 | 525 |
| 026 | 974 | -959 | -816 | -588 | -297 | 025 | 345 | 628 | 844 | 972 | 996 | 474 | 526 |
| 027 | 973 | -913 | -725 | -454 | -132 | 206 | 520 | 775 | 941 | 1000 | 945 | 473 | 527 |
| 028 | 972 | -851 | -618 | -309 | 038 | 380 | 675 | 888 | 992 | 975 | 838 | 472 | 528 |
| 029 | 971 | -775 | -498 | -156 | 206 | 541 | 805 | 964 | 996 | 897 | 680 | 471 | 529 |
| | | | | | | | | | | | | | |
| 030 | 970 | -685 | -368 | 000 | 368 | 685 | 905 | 998 | 951 | 771 | 482 | 470 | 530 |
| 031 | 969 | -583 | -230 | 156 | 520 | 805 | 970 | 990 | 861 | 603 | 255 | 469 | 531 |
| 032 | 968 | -471 | -088 | 309 | 657 | 899 | 999 | 939 | 729 | 403 | 013 | 468 | 532 |
| 033 | 967 | -351 | 057 | 454 | 775 | 964 | 990 | 848 | 562 | 181 | -230 | 467 | 533 |
| 034 | 966 | -224 | 200 | 588 | 870 | 996 | 943 | 720 | 368 | -050 | -460 | 466 | 534 |
| | | | | | | | | | | | | | |
| 035 | 965 | -094 | 339 | 707 | 941 | 996 | 861 | 562 | 156 | -279 | -661 | 465 | 535 |
| 036 | 964 | 038 | 471 | 809 | 985 | 962 | 746 | 380 | -063 | -493 | -824 | 464 | 536 |
| 037 | 963 | 169 | 593 | 891 | 1000 | 897 | 603 | 181 | -279 | -680 | -937 | 463 | 537 |
| 038 | 962 | 297 | 703 | 951 | 987 | 802 | 437 | -025 | -482 | -831 | -994 | 462 | 538 |
| 039 | 961 | 420 | 798 | 988 | 945 | 680 | 255 | -230 | -661 | -937 | -991 | 461 | 539 |
| | | | | | | | | | | | | | |
| 040 | 960 | 536 | 876 | 1000 | 876 | 536 | 063 | -426 | -809 | -992 | -930 | 460 | 540 |
| 041 | 959 | 642 | 937 | 988 | 782 | 374 | -132 | -603 | -918 | -994 | -813 | 459 | 541 |
| 042 | 958 | 737 | 977 | 951 | 666 | 200 | -321 | -754 | -982 | -943 | -647 | 458 | 542 |
| 043 | 957 | 820 | 998 | 891 | 531 | 019 | -498 | -873 | -1000 | -841 | -443 | 457 | 543 |
| 044 | 956 | 888 | 997 | 809 | 380 | -163 | -657 | -955 | -969 | -694 | -212 | 456 | 544 |

TABLE 8.5C (continued)
 $\cos 2\pi hx$ (h odd) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=1$ | 3 | 5 | 7 | 9 | 11 | 13 | 15 | 17 | 19 | Change sign.
x | |
|-----------------------|-----|-------|------|------|-------|-------|-------|------|------|-------|-------|---------------------|-----|
| 045 | 955 | 960 | 661 | 156 | -397 | -827 | -1000 | -861 | -454 | 094 | 613 | 455 | 545 |
| 046 | 954 | 959 | 647 | 125 | -437 | -858 | -999 | -816 | -368 | 200 | 703 | 454 | 546 |
| 047 | 953 | 957 | 633 | 094 | -476 | -885 | -994 | -767 | -279 | 303 | 782 | 453 | 547 |
| 048 | 952 | 955 | 618 | 063 | -514 | -910 | -985 | -712 | -187 | 403 | 851 | 452 | 548 |
| 049 | 951 | 953 | 603 | 031 | -552 | -932 | -970 | -652 | -094 | 498 | 907 | 451 | 549 |
| | | | | | | | | | | | | | |
| 050 | 950 | 951 | 588 | 000 | -588 | -951 | -951 | -588 | 000 | 588 | 951 | 450 | 550 |
| 051 | 949 | 949 | 572 | -031 | -623 | -967 | -927 | -520 | 094 | 671 | 981 | 449 | 551 |
| 052 | 948 | 947 | 557 | -063 | -657 | -980 | -899 | -448 | 187 | 746 | 997 | 448 | 552 |
| 053 | 947 | 945 | 541 | -094 | -689 | -990 | -867 | -374 | 279 | 813 | 999 | 447 | 553 |
| 054 | 946 | 943 | 525 | -125 | -720 | -996 | -831 | -297 | 368 | 870 | 987 | 446 | 554 |
| | | | | | | | | | | | | | |
| 055 | 945 | 941 | 509 | -156 | -750 | -1000 | -790 | -218 | 454 | 918 | 960 | 445 | 555 |
| 056 | 944 | 939 | 493 | -187 | -778 | -1000 | -746 | -138 | 536 | 955 | 920 | 444 | 556 |
| 057 | 943 | 937 | 476 | -218 | -805 | -997 | -698 | -057 | 613 | 981 | 867 | 443 | 557 |
| 058 | 942 | 934 | 460 | -249 | -831 | -990 | -647 | 025 | 685 | 996 | 802 | 442 | 558 |
| 059 | 941 | 932 | 443 | -279 | -854 | -981 | -593 | 107 | 750 | 1000 | 725 | 441 | 559 |
| | | | | | | | | | | | | | |
| 060 | 940 | 930 | 426 | -309 | -876 | -969 | -536 | 187 | 809 | 992 | 637 | 440 | 560 |
| 061 | 939 | 927 | 409 | -339 | -897 | -953 | -476 | 267 | 861 | 973 | 541 | 439 | 561 |
| 062 | 938 | 925 | 391 | -368 | -915 | -934 | -414 | 345 | 905 | 943 | 437 | 438 | 562 |
| 063 | 937 | 923 | 374 | -397 | -932 | -913 | -351 | 420 | 941 | 902 | 327 | 437 | 563 |
| 064 | 936 | 920 | 356 | -426 | -947 | -888 | -285 | 493 | 969 | 851 | 212 | 436 | 564 |
| | | | | | | | | | | | | | |
| 065 | 935 | 918 | 339 | -454 | -960 | -861 | -218 | 562 | 988 | 790 | 094 | 435 | 565 |
| 066 | 934 | 915 | 321 | -482 | -972 | -831 | -150 | 628 | 998 | 720 | -025 | 434 | 566 |
| 067 | 933 | 913 | 303 | -509 | -981 | -798 | -082 | 689 | 1000 | 642 | -144 | 433 | 567 |
| 068 | 932 | 910 | 285 | -536 | -989 | -762 | -013 | 746 | 992 | 557 | -261 | 432 | 568 |
| 069 | 931 | 907 | 267 | -562 | -994 | -725 | 057 | 798 | 976 | 465 | -374 | 431 | 569 |
| | | | | | | | | | | | | | |
| 070 | 930 | 905 | 249 | -588 | -998 | -685 | 125 | 844 | 951 | 368 | -482 | 430 | 570 |
| 071 | 929 | 902 | 230 | -613 | -1000 | -642 | 194 | 885 | 918 | 267 | -583 | 429 | 571 |
| 072 | 928 | 899 | 212 | -637 | -1000 | -598 | 261 | 920 | 876 | 163 | -675 | 428 | 572 |
| 073 | 927 | 897 | 194 | -661 | -998 | -552 | 327 | 949 | 827 | 057 | -758 | 427 | 573 |
| 074 | 926 | 894 | 175 | -685 | -994 | -504 | 391 | 972 | 771 | -050 | -831 | 426 | 574 |
| | | | | | | | | | | | | | |
| 075 | 925 | 891 | 156 | -707 | -988 | -454 | 454 | 988 | 707 | -156 | -891 | 425 | 575 |
| 076 | 924 | 888 | 138 | -729 | -980 | -403 | 514 | 997 | 637 | -261 | -939 | 424 | 576 |
| 077 | 923 | 885 | 119 | -750 | -970 | -351 | 572 | 1000 | 562 | -362 | -973 | 423 | 577 |
| 078 | 922 | 882 | 100 | -771 | -959 | -297 | 628 | 996 | 482 | -460 | -994 | 422 | 578 |
| 079 | 921 | 879 | 082 | -790 | -945 | -243 | 680 | 986 | 397 | -552 | -1000 | 421 | 579 |
| | | | | | | | | | | | | | |
| 080 | 920 | 876 | 063 | -809 | -930 | -187 | 729 | 969 | 309 | -637 | -992 | 420 | 580 |
| 081 | 919 | 873 | 044 | -827 | -913 | -132 | 775 | 945 | 218 | -716 | -970 | 419 | 581 |
| 082 | 918 | 870 | 025 | -844 | -894 | -075 | 816 | 915 | 125 | -786 | -934 | 418 | 582 |
| 083 | 917 | 867 | 006 | -861 | -873 | -019 | 854 | 879 | 031 | -848 | -885 | 417 | 583 |
| 084 | 916 | 864 | -013 | -876 | -851 | 038 | 888 | 838 | -063 | -899 | -824 | 416 | 584 |
| | | | | | | | | | | | | | |
| 085 | 915 | 861 | -031 | -891 | -827 | 094 | 918 | 790 | -156 | -941 | -750 | 415 | 585 |
| 086 | 914 | 858 | -050 | -905 | -802 | 150 | 943 | 738 | -249 | -972 | -666 | 414 | 586 |
| 087 | 913 | 854 | -069 | -918 | -775 | 206 | 964 | 680 | -339 | -991 | -572 | 413 | 587 |
| 088 | 912 | 851 | -088 | -930 | -746 | 261 | 980 | 618 | -426 | -1000 | -471 | 412 | 588 |
| 089 | 911 | 848 | -107 | -941 | -716 | 315 | 991 | 552 | -509 | -997 | -362 | 411 | 589 |

TABLE 8.5C (continued)

 $\cos 2\pi hx$ (h odd) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=21$ | 23 | 25 | 27 | 29 | 31 | 33 | 35 | 37 | 39 | Change sign:
x | |
|-----------------------|-----|--------|-------|-------|------|------|------|------|------|------|-------|---------------------|-----|
| 045 | 955 | 941 | 976 | 707 | 218 | -339 | -790 | -996 | -891 | -509 | 031 | 455 | 545 |
| 046 | 954 | 977 | 934 | 588 | 050 | -504 | -894 | -994 | -771 | -297 | 273 | 454 | 546 |
| 047 | 953 | 997 | 873 | 454 | -119 | -652 | -964 | -949 | -613 | -069 | 498 | 453 | 547 |
| 048 | 952 | 999 | 794 | 309 | -285 | -778 | -997 | -864 | -426 | 163 | 694 | 452 | 548 |
| 049 | 951 | 983 | 698 | 156 | -443 | -879 | -993 | -742 | -218 | 386 | 848 | 451 | 549 |
| 050 | 950 | 951 | 588 | 000 | -588 | -951 | -951 | -588 | 000 | 588 | 951 | 450 | 550 |
| 051 | 949 | 902 | 465 | -156 | -716 | -991 | -873 | -409 | 218 | 758 | 998 | 449 | 551 |
| 052 | 948 | 838 | 333 | -309 | -824 | -999 | -762 | -212 | 426 | 888 | 985 | 448 | 552 |
| 053 | 947 | 758 | 194 | -454 | -907 | -973 | -623 | -006 | 613 | 970 | 913 | 447 | 553 |
| 054 | 946 | 666 | 050 | -588 | -965 | -915 | -460 | 200 | 771 | 1000 | 786 | 446 | 554 |
| 055 | 945 | 562 | -094 | -707 | -996 | -827 | -279 | 397 | 891 | 976 | 613 | 445 | 555 |
| 056 | 944 | 448 | -237 | -809 | -997 | -712 | -088 | 578 | 969 | 899 | 403 | 444 | 556 |
| 057 | 943 | 327 | -374 | -891 | -970 | -572 | 107 | 733 | 1000 | 775 | 169 | 443 | 557 |
| 058 | 942 | 200 | -504 | -951 | -915 | -414 | 297 | 858 | 982 | 608 | -075 | 442 | 558 |
| 059 | 941 | 069 | -623 | -988 | -834 | -243 | 476 | 945 | 918 | 409 | -315 | 441 | 559 |
| 060 | 940 | -063 | -729 | -1000 | -729 | -063 | 637 | 992 | 809 | 187 | -536 | 440 | 560 |
| 061 | 939 | -194 | -820 | -988 | -603 | 119 | 775 | 997 | 661 | -044 | -725 | 439 | 561 |
| 062 | 938 | -321 | -894 | -951 | -460 | 297 | 882 | 959 | 482 | -273 | -870 | 438 | 562 |
| 063 | 937 | -443 | -949 | -891 | -303 | 465 | 957 | 879 | 279 | -487 | -964 | 437 | 563 |
| 064 | 936 | -557 | -985 | -809 | -138 | 618 | 995 | 762 | 063 | -675 | -1000 | 436 | 564 |
| 065 | 935 | -661 | -1000 | -707 | 031 | 750 | 996 | 613 | -156 | -827 | -976 | 435 | 565 |
| 066 | 934 | -754 | -994 | -588 | 200 | 858 | 959 | 437 | -368 | -934 | -894 | 434 | 566 |
| 067 | 933 | -834 | -967 | -454 | 362 | 937 | 885 | 243 | -562 | -991 | -758 | 433 | 567 |
| 068 | 932 | -899 | -920 | -309 | 514 | 985 | 778 | 038 | -729 | -995 | -578 | 432 | 568 |
| 069 | 931 | -949 | -854 | -156 | 652 | 1000 | 642 | -169 | -861 | -945 | -362 | 431 | 569 |
| 070 | 930 | -982 | -771 | 000 | 771 | 982 | 482 | -368 | -951 | -844 | -125 | 430 | 570 |
| 071 | 929 | -998 | -671 | 156 | 867 | 932 | 303 | -552 | -996 | -698 | 119 | 429 | 571 |
| 072 | 928 | -997 | -557 | 309 | 939 | 851 | 113 | -712 | -992 | -514 | 356 | 428 | 572 |
| 073 | 927 | -979 | -431 | 454 | 983 | 742 | -082 | -841 | -941 | -303 | 572 | 427 | 573 |
| 074 | 926 | -943 | -297 | 588 | 1000 | 608 | -273 | -934 | -844 | -075 | 754 | 426 | 574 |
| 075 | 925 | -891 | -156 | 707 | 988 | 454 | -454 | -988 | -707 | 156 | 891 | 425 | 575 |
| 076 | 924 | -824 | -013 | 809 | 947 | 285 | -618 | -999 | -536 | 380 | 975 | 424 | 576 |
| 077 | 923 | -742 | 132 | 891 | 879 | 107 | -758 | -967 | -339 | 583 | 1000 | 423 | 577 |
| 078 | 922 | -647 | 273 | 951 | 786 | -075 | -870 | -894 | -125 | 754 | 965 | 422 | 578 |
| 079 | 921 | -541 | 409 | 988 | 671 | -255 | -949 | -782 | 094 | 885 | 873 | 421 | 579 |
| 080 | 920 | -426 | 536 | 1000 | 536 | -426 | -992 | -637 | 309 | 969 | 729 | 420 | 580 |
| 081 | 919 | -303 | 652 | 988 | 386 | -583 | -998 | -465 | 509 | 1000 | 541 | 419 | 581 |
| 082 | 918 | -175 | 754 | 951 | 224 | -720 | -965 | -273 | 685 | 977 | 321 | 418 | 582 |
| 083 | 917 | -044 | 841 | 891 | 057 | -834 | -897 | -069 | 827 | 902 | 082 | 417 | 583 |
| 084 | 916 | 088 | 910 | 809 | -113 | -920 | -794 | 138 | 930 | 778 | -163 | 416 | 584 |
| 085 | 915 | 218 | 960 | 707 | -279 | -976 | -661 | 339 | 988 | 613 | -397 | 415 | 585 |
| 086 | 914 | 345 | 990 | 588 | -437 | -999 | -504 | 525 | 998 | 414 | -608 | 414 | 586 |
| 087 | 913 | 465 | 1000 | 454 | -583 | -990 | -327 | 689 | 960 | 194 | -782 | 413 | 587 |
| 088 | 912 | 578 | 989 | 309 | -712 | -947 | -138 | 824 | 876 | -038 | -910 | 412 | 588 |
| 089 | 911 | 680 | 957 | 156 | -820 | -873 | 057 | 923 | 750 | -267 | -983 | 411 | 589 |

TABLE 8.5C (continued)

 $\cos 2\pi hx$ (h odd) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=1$ | 3 | 5 | 7 | 9 | 11 | 13 | 15 | 17 | 19 | Change sign.
x | |
|-----------------------|-----|-------|------|-------|------|------|------|-------|-------|------|------|---------------------|-----|
| 090 | 910 | 844 | -125 | -951 | -685 | 368 | 998 | 482 | -588 | -982 | -249 | 410 | 590 |
| 091 | 909 | 841 | -144 | -960 | -652 | 420 | 1000 | 409 | -661 | -957 | -132 | 409 | 591 |
| 092 | 908 | 838 | -163 | -969 | -618 | 471 | 997 | 333 | -729 | -920 | -013 | 408 | 592 |
| 093 | 907 | 834 | -181 | -976 | -583 | 520 | 990 | 255 | -790 | -873 | 107 | 407 | 593 |
| 094 | 906 | 831 | -200 | -982 | -546 | 567 | 977 | 175 | -844 | -816 | 224 | 406 | 594 |
| 095 | 905 | 827 | -218 | -988 | -509 | 613 | 960 | 094 | -891 | -750 | 339 | 405 | 595 |
| 096 | 904 | 824 | -237 | -992 | -471 | 657 | 939 | 013 | -930 | -675 | 448 | 404 | 596 |
| 097 | 903 | 820 | -255 | -996 | -431 | 698 | 913 | -069 | -960 | -593 | 552 | 403 | 597 |
| 098 | 902 | 816 | -273 | -998 | -391 | 737 | 882 | -150 | -982 | -504 | 647 | 402 | 598 |
| 099 | 901 | 813 | -291 | -1000 | -351 | 775 | 848 | -230 | -996 | -409 | 733 | 401 | 599 |
| 100 | 900 | 809 | -309 | -1000 | -309 | 809 | 809 | -309 | -1000 | -309 | 809 | 400 | 600 |
| 101 | 899 | 805 | -327 | -1000 | -267 | 841 | 767 | -386 | -996 | -206 | 873 | 399 | 601 |
| 102 | 898 | 802 | -345 | -998 | -224 | 870 | 720 | -460 | -982 | -100 | 925 | 398 | 602 |
| 103 | 897 | 798 | -362 | -996 | -181 | 897 | 671 | -531 | -960 | 006 | 964 | 397 | 603 |
| 104 | 896 | 794 | -380 | -992 | -138 | 920 | 618 | -598 | -930 | 113 | 989 | 396 | 604 |
| 105 | 895 | 790 | -397 | -988 | -094 | 941 | 562 | -661 | -891 | 218 | 1000 | 395 | 605 |
| 106 | 894 | 786 | -414 | -982 | -050 | 959 | 504 | -720 | -844 | 321 | 996 | 394 | 606 |
| 107 | 893 | 782 | -431 | -976 | -006 | 973 | 443 | -775 | -790 | 420 | 979 | 393 | 607 |
| 108 | 892 | 778 | -448 | -969 | 038 | 985 | 380 | -824 | -729 | 514 | 947 | 392 | 608 |
| 109 | 891 | 775 | -465 | -960 | 082 | 993 | 315 | -867 | -661 | 603 | 902 | 391 | 609 |
| 110 | 890 | 771 | -482 | -951 | 125 | 998 | 249 | -905 | -588 | 685 | 844 | 390 | 610 |
| 111 | 889 | 767 | -498 | -941 | 169 | 1000 | 181 | -937 | -509 | 758 | 775 | 389 | 611 |
| 112 | 888 | 762 | -514 | -930 | 212 | 999 | 113 | -962 | -426 | 824 | 694 | 388 | 612 |
| 113 | 887 | 758 | -531 | -918 | 255 | 994 | 044 | -981 | -339 | 879 | 603 | 387 | 613 |
| 114 | 886 | 754 | -546 | -905 | 297 | 987 | -025 | -994 | -249 | 925 | 504 | 386 | 614 |
| 115 | 885 | 750 | -562 | -891 | 339 | 976 | -094 | -1000 | -156 | 960 | 397 | 385 | 615 |
| 116 | 884 | 746 | -578 | -876 | 380 | 962 | -163 | -999 | -063 | 985 | 285 | 384 | 616 |
| 117 | 883 | 742 | -593 | -861 | 420 | 945 | -230 | -991 | 031 | 998 | 169 | 383 | 617 |
| 118 | 882 | 738 | -608 | -844 | 460 | 925 | -297 | -977 | 125 | 999 | 050 | 382 | 618 |
| 119 | 881 | 733 | -623 | -827 | 498 | 902 | -362 | -957 | 218 | 990 | -069 | 381 | 619 |
| 120 | 880 | 729 | -637 | -809 | 536 | 876 | -426 | -930 | 309 | 969 | -187 | 380 | 620 |
| 121 | 879 | 725 | -652 | -790 | 572 | 848 | -487 | -897 | 397 | 937 | -303 | 379 | 621 |
| 122 | 878 | 720 | -666 | -771 | 608 | 816 | -546 | -858 | 482 | 894 | -414 | 378 | 622 |
| 123 | 877 | 716 | -680 | -750 | 642 | 782 | -603 | -813 | 562 | 841 | -520 | 377 | 623 |
| 124 | 876 | 712 | -694 | -729 | 675 | 746 | -657 | -762 | 637 | 778 | -618 | 376 | 624 |
| 125 | 875 | 707 | -707 | -707 | 707 | 707 | -707 | -707 | 707 | 707 | -707 | 375 | 625 |
| 126 | 874 | 703 | -720 | -685 | 737 | 666 | -754 | -647 | 771 | 628 | -786 | 374 | 626 |
| 127 | 873 | 698 | -733 | -661 | 767 | 623 | -798 | -583 | 827 | 541 | -854 | 373 | 627 |
| 128 | 872 | 694 | -746 | -637 | 794 | 578 | -838 | -514 | 876 | 448 | -910 | 372 | 628 |
| 129 | 871 | 689 | -758 | -613 | 820 | 531 | -873 | -443 | 918 | 351 | -953 | 371 | 629 |
| 130 | 870 | 685 | -771 | -588 | 844 | 482 | -905 | -368 | 951 | 249 | -982 | 370 | 630 |
| 131 | 869 | 680 | -782 | -562 | 867 | 431 | -932 | -291 | 976 | 144 | -998 | 369 | 631 |
| 132 | 868 | 675 | -794 | -536 | 888 | 380 | -955 | -212 | 992 | 038 | -999 | 368 | 632 |
| 133 | 867 | 671 | -805 | -509 | 907 | 327 | -973 | -132 | 1000 | -069 | -986 | 367 | 633 |
| 134 | 866 | 666 | -816 | -482 | 925 | 273 | -987 | -050 | 998 | -175 | -959 | 366 | 634 |

TABLE 8.5C (*continued*)
 $\cos 2\pi hx$ (h odd) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=21$ | 23 | 25 | 27 | 29 | 31 | 33 | 35 | 37 | 39 | Change sign.
x | |
|-----------------------|-----|--------|------|-------|------|------|-------|-------|-------|------|------|---------------------|-----|
| 090 | 910 | 771 | 905 | 000 | −905 | −771 | 249 | 982 | 588 | −482 | −998 | 410 | 590 |
| 091 | 909 | 848 | 834 | −156 | −964 | −642 | 431 | 1000 | 397 | −671 | −953 | 409 | 591 |
| 092 | 908 | 910 | 746 | −309 | −995 | −493 | 598 | 975 | 187 | −824 | −851 | 408 | 592 |
| 093 | 907 | 957 | 642 | −454 | −998 | −327 | 742 | 907 | −031 | −932 | −698 | 407 | 593 |
| 094 | 906 | 987 | 525 | −588 | −972 | −150 | 858 | 802 | −249 | −990 | −504 | 406 | 594 |
| | | | | | | | | | | | | | |
| 095 | 905 | 1000 | 397 | −707 | −918 | 031 | 941 | 661 | −454 | −996 | −279 | 405 | 595 |
| 096 | 904 | 995 | 261 | −809 | −838 | 212 | 989 | 493 | −637 | −947 | −038 | 404 | 596 |
| 097 | 903 | 973 | 119 | −891 | −733 | 386 | 999 | 303 | −790 | −848 | 206 | 403 | 597 |
| 098 | 902 | 934 | −025 | −951 | −608 | 546 | 972 | 100 | −905 | −703 | 437 | 402 | 598 |
| 099 | 901 | 879 | −169 | −988 | −465 | 689 | 907 | −107 | −976 | −520 | 642 | 401 | 599 |
| | | | | | | | | | | | | | |
| 100 | 900 | 809 | −309 | −1000 | −309 | 809 | 809 | −309 | −1000 | −309 | 809 | 400 | 600 |
| 101 | 899 | 725 | −443 | −988 | −144 | 902 | 680 | −498 | −976 | −082 | 927 | 399 | 601 |
| 102 | 898 | 628 | −567 | −951 | 025 | 965 | 525 | −666 | −905 | 150 | 990 | 398 | 602 |
| 103 | 897 | 520 | −680 | −891 | 194 | 997 | 351 | −805 | −790 | 374 | 994 | 397 | 603 |
| 104 | 896 | 403 | −778 | −809 | 356 | 995 | 163 | −910 | −637 | 578 | 939 | 396 | 604 |
| | | | | | | | | | | | | | |
| 105 | 895 | 279 | −861 | −707 | 509 | 960 | −031 | −976 | −454 | 750 | 827 | 395 | 605 |
| 106 | 894 | 150 | −925 | −588 | 647 | 894 | −224 | −1000 | −249 | 882 | 666 | 394 | 606 |
| 107 | 893 | 019 | −970 | −454 | 767 | 798 | −409 | −981 | −031 | 967 | 465 | 393 | 607 |
| 108 | 892 | −113 | −995 | −309 | 864 | 675 | −578 | −920 | 187 | 1000 | 237 | 392 | 608 |
| 109 | 891 | −243 | −999 | −156 | 937 | 531 | −725 | −820 | 397 | 979 | −006 | 391 | 609 |
| | | | | | | | | | | | | | |
| 110 | 890 | −368 | −982 | 000 | 982 | 368 | −844 | −685 | 588 | 905 | −249 | 390 | 610 |
| 111 | 889 | −487 | −945 | 156 | 1000 | 194 | −932 | −520 | 750 | 782 | −476 | 389 | 611 |
| 112 | 888 | −598 | −888 | 309 | 989 | 013 | −985 | −333 | 876 | 618 | −675 | 388 | 612 |
| 113 | 887 | −698 | −813 | 454 | 949 | −169 | −1000 | −132 | 960 | 420 | −834 | 387 | 613 |
| 114 | 886 | −786 | −720 | 588 | 882 | −345 | −977 | 075 | 998 | 200 | −943 | 386 | 614 |
| | | | | | | | | | | | | | |
| 115 | 885 | −861 | −613 | 707 | 790 | −509 | −918 | 279 | 988 | −031 | −996 | 385 | 615 |
| 116 | 884 | −920 | −493 | 809 | 675 | −657 | −824 | 471 | 930 | −261 | −989 | 384 | 616 |
| 117 | 883 | −964 | −362 | 891 | 541 | −782 | −698 | 642 | 827 | −476 | −923 | 383 | 617 |
| 118 | 882 | −990 | −224 | 951 | 391 | −882 | −546 | 786 | 685 | −666 | −802 | 382 | 618 |
| 119 | 881 | −1000 | −082 | 988 | 230 | −953 | −374 | 897 | 509 | −820 | −633 | 381 | 619 |
| | | | | | | | | | | | | | |
| 120 | 880 | −992 | 063 | 1000 | 063 | −992 | −187 | 969 | 309 | −930 | −426 | 380 | 620 |
| 121 | 879 | −967 | 206 | 988 | −107 | −998 | 006 | 999 | 094 | −990 | −194 | 379 | 621 |
| 122 | 878 | −925 | 345 | 951 | −273 | −972 | 200 | 987 | −125 | −996 | 050 | 378 | 622 |
| 123 | 877 | −867 | 476 | 891 | −431 | −913 | 386 | 932 | −339 | −949 | 291 | 377 | 623 |
| 124 | 876 | −794 | 598 | 809 | −578 | −824 | 557 | 838 | −536 | −851 | 514 | 376 | 624 |
| | | | | | | | | | | | | | |
| 125 | 875 | −707 | 707 | 707 | −707 | −707 | 707 | 707 | −707 | −707 | 707 | 375 | 625 |
| 126 | 874 | −608 | 802 | 588 | −816 | −567 | 831 | 546 | −844 | −525 | 858 | 374 | 626 |
| 127 | 873 | −498 | 879 | 454 | −902 | −409 | 923 | 362 | −941 | −315 | 957 | 373 | 627 |
| 128 | 872 | −380 | 939 | 309 | −962 | −237 | 980 | 163 | −992 | −088 | 999 | 372 | 628 |
| 129 | 871 | −255 | 979 | 156 | −994 | −057 | 1000 | −044 | −996 | 144 | 981 | 371 | 629 |
| | | | | | | | | | | | | | |
| 130 | 870 | −125 | 998 | 000 | −998 | 125 | 982 | −249 | −951 | 368 | 905 | 370 | 630 |
| 131 | 869 | 006 | 997 | −156 | −973 | 303 | 927 | −443 | −861 | 572 | 775 | 369 | 631 |
| 132 | 868 | 138 | 975 | −309 | −920 | 471 | 838 | −618 | −729 | 746 | 598 | 368 | 632 |
| 133 | 867 | 267 | 932 | −454 | −841 | 623 | 716 | −767 | −562 | 879 | 386 | 367 | 633 |
| 134 | 866 | 391 | 870 | −588 | −738 | 754 | 567 | −882 | −368 | 965 | 150 | 366 | 634 |

TABLE 8.5C (*continued*)
 $\cos 2\pi hx$ (h odd) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=1$ | 3 | 5 | 7 | 9 | 11 | 13 | 15 | 17 | 19 | Change sign.
x | |
|-----------------------|-----|-------|-------|------|------|-------|-------|------|-------|-------|------|---------------------|-----|
| 135 | 865 | 661 | -827 | -454 | 941 | 218 | -996 | 031 | 988 | -279 | -918 | 365 | 635 |
| 136 | 864 | 657 | -838 | -426 | 955 | 163 | -1000 | 113 | 969 | -380 | -864 | 364 | 636 |
| 137 | 863 | 652 | -848 | -397 | 967 | 107 | -999 | 194 | 941 | -476 | -798 | 363 | 637 |
| 138 | 862 | 647 | -858 | -368 | 977 | 050 | -994 | 273 | 905 | -567 | -720 | 362 | 638 |
| 139 | 861 | 642 | -867 | -339 | 986 | -006 | -983 | 351 | 861 | -652 | -633 | 361 | 639 |
| | | | | | | | | | | | | | |
| 140 | 860 | 637 | -876 | -309 | 992 | -063 | -969 | 426 | 809 | -729 | -536 | 360 | 640 |
| 141 | 859 | 633 | -885 | -279 | 997 | -119 | -949 | 498 | 750 | -798 | -431 | 359 | 641 |
| 142 | 858 | 628 | -894 | -249 | 999 | -175 | -925 | 567 | 685 | -858 | -321 | 358 | 642 |
| 143 | 857 | 623 | -902 | -218 | 1000 | -230 | -897 | 633 | 613 | -907 | -206 | 357 | 643 |
| 144 | 856 | 618 | -910 | -187 | 999 | -285 | -864 | 694 | 536 | -947 | -088 | 356 | 644 |
| | | | | | | | | | | | | | |
| 145 | 855 | 613 | -918 | -156 | 996 | -339 | -827 | 750 | 454 | -976 | 031 | 355 | 645 |
| 146 | 854 | 608 | -925 | -125 | 990 | -391 | -786 | 802 | 368 | -994 | 150 | 354 | 646 |
| 147 | 853 | 603 | -932 | -094 | 983 | -443 | -742 | 848 | 279 | -1000 | 267 | 353 | 647 |
| 148 | 852 | 598 | -939 | -063 | 975 | -493 | -694 | 888 | 187 | -995 | 380 | 352 | 648 |
| 149 | 851 | 593 | -945 | -031 | 964 | -541 | -642 | 923 | 094 | -979 | 487 | 351 | 649 |
| | | | | | | | | | | | | | |
| 150 | 850 | 588 | -951 | 000 | 951 | -588 | -588 | 951 | 000 | -951 | 588 | 350 | 650 |
| 151 | 849 | 583 | -957 | 031 | 937 | -633 | -531 | 973 | -094 | -913 | 680 | 349 | 651 |
| 152 | 848 | 578 | -962 | 063 | 920 | -675 | -471 | 989 | -187 | -864 | 762 | 348 | 652 |
| 153 | 847 | 572 | -967 | 094 | 902 | -716 | -409 | 998 | -279 | -805 | 834 | 347 | 653 |
| 154 | 846 | 567 | -972 | 125 | 882 | -754 | -345 | 1000 | -368 | -738 | 894 | 346 | 654 |
| | | | | | | | | | | | | | |
| 155 | 845 | 562 | -976 | 156 | 861 | -790 | -279 | 996 | -454 | -661 | 941 | 345 | 655 |
| 156 | 844 | 557 | -980 | 187 | 838 | -824 | -212 | 985 | -536 | -578 | 975 | 344 | 656 |
| 157 | 843 | 552 | -983 | 218 | 813 | -854 | -144 | 967 | -613 | -487 | 994 | 343 | 657 |
| 158 | 842 | 546 | -987 | 249 | 786 | -882 | -075 | 943 | -685 | -391 | 1000 | 342 | 658 |
| 159 | 841 | 541 | -990 | 279 | 758 | -907 | -006 | 913 | -750 | -291 | 991 | 341 | 659 |
| | | | | | | | | | | | | | |
| 160 | 840 | 536 | -992 | 309 | 729 | -930 | 063 | 876 | -809 | -187 | 969 | 340 | 660 |
| 161 | 839 | 531 | -994 | 339 | 698 | -949 | 132 | 834 | -861 | -082 | 932 | 339 | 661 |
| 162 | 838 | 525 | -996 | 368 | 666 | -965 | 200 | 786 | -905 | 025 | 882 | 338 | 662 |
| 163 | 837 | 520 | -998 | 397 | 633 | -979 | 267 | 733 | -941 | 132 | 820 | 337 | 663 |
| 164 | 836 | 514 | -999 | 426 | 598 | -989 | 333 | 675 | -969 | 237 | 746 | 336 | 664 |
| | | | | | | | | | | | | | |
| 165 | 835 | 509 | -1000 | 454 | 562 | -996 | 397 | 613 | -988 | 339 | 661 | 335 | 665 |
| 166 | 834 | 504 | -1000 | 482 | 525 | -999 | 460 | 546 | -998 | 437 | 567 | 334 | 666 |
| 167 | 833 | 498 | -1000 | 509 | 487 | -1000 | 520 | 476 | -1000 | 531 | 465 | 333 | 667 |
| 168 | 832 | 493 | -1000 | 536 | 448 | -997 | 578 | 403 | -992 | 618 | 356 | 332 | 668 |
| 169 | 831 | 487 | -999 | 562 | 409 | -991 | 633 | 327 | -976 | 698 | 243 | 331 | 669 |
| | | | | | | | | | | | | | |
| 170 | 830 | 482 | -998 | 588 | 368 | -982 | 685 | 249 | -951 | 771 | 125 | 330 | 670 |
| 171 | 829 | 476 | -997 | 613 | 327 | -970 | 733 | 169 | -918 | 834 | 006 | 329 | 671 |
| 172 | 828 | 471 | -995 | 637 | 285 | -955 | 778 | 088 | -876 | 888 | -113 | 328 | 672 |
| 173 | 827 | 465 | -993 | 661 | 243 | -937 | 820 | 006 | -827 | 932 | -230 | 327 | 673 |
| 174 | 826 | 460 | -990 | 685 | 200 | -915 | 858 | -075 | -771 | 965 | -345 | 326 | 674 |
| | | | | | | | | | | | | | |
| 175 | 825 | 454 | -988 | 707 | 156 | -891 | 891 | -156 | -707 | 988 | -454 | 325 | 675 |
| 176 | 824 | 448 | -985 | 729 | 113 | -864 | 920 | -237 | -637 | 999 | -557 | 324 | 676 |
| 177 | 823 | 443 | -981 | 750 | 069 | -834 | 945 | -315 | -562 | 998 | -652 | 323 | 677 |
| 178 | 822 | 437 | -977 | 771 | 025 | -802 | 965 | -391 | -482 | 987 | -738 | 322 | 678 |
| 179 | 821 | 431 | -973 | 790 | -019 | -767 | 981 | -465 | -397 | 964 | -813 | 321 | 679 |

TABLE 8.5C (continued)

 $\cos 2\pi hx$ (h odd) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=21$ | 23 | 25 | 27 | 29 | 31 | 33 | 35 | 37 | 39 | Change sign.
x | |
|-----------------------|-----|--------|-------|-------|------|-------|-------|------|-------|------|-------|---------------------|-----|
| 135 | 865 | 509 | 790 | -707 | -613 | 861 | 397 | -960 | -156 | 1000 | -094 | 365 | 635 |
| 136 | 864 | 618 | 694 | -809 | -471 | 939 | 212 | -997 | 063 | 980 | -333 | 364 | 636 |
| 137 | 863 | 716 | 583 | -891 | -315 | 986 | 019 | -991 | 279 | 907 | -552 | 363 | 637 |
| 138 | 862 | 802 | 460 | -951 | -150 | 1000 | -175 | -943 | 482 | 786 | -738 | 362 | 638 |
| 139 | 861 | 873 | 327 | -988 | 019 | 981 | -362 | -854 | 661 | 623 | -879 | 361 | 639 |
| 140 | 860 | 930 | 187 | -1000 | 187 | 930 | -536 | -729 | 809 | 426 | -969 | 360 | 640 |
| 141 | 859 | 970 | 044 | -988 | 351 | 848 | -689 | -572 | 918 | 206 | -1000 | 359 | 641 |
| 142 | 858 | 994 | -100 | -951 | 504 | 738 | -816 | -391 | 982 | -025 | -972 | 358 | 642 |
| 143 | 857 | 1000 | -243 | -891 | 642 | 603 | -913 | -194 | 1000 | -255 | -885 | 357 | 643 |
| 144 | 856 | 989 | -380 | -809 | 762 | 448 | -975 | 013 | 969 | -471 | -746 | 356 | 644 |
| 145 | 855 | 960 | -509 | -707 | 861 | 279 | -1000 | 218 | 891 | -661 | -562 | 355 | 645 |
| 146 | 854 | 915 | -628 | -588 | 934 | 100 | -987 | 414 | 771 | -816 | -345 | 354 | 646 |
| 147 | 853 | 854 | -733 | -454 | 981 | -082 | -937 | 593 | 613 | -927 | -107 | 353 | 647 |
| 148 | 852 | 778 | -824 | -309 | 1000 | -261 | -851 | 746 | 426 | -989 | 138 | 352 | 648 |
| 149 | 851 | 689 | -897 | -156 | 990 | -431 | -733 | 867 | 218 | -997 | 374 | 351 | 649 |
| 150 | 850 | 588 | -951 | 000 | 951 | -588 | -588 | 951 | 000 | -951 | 588 | 350 | 650 |
| 151 | 849 | 476 | -986 | 156 | 885 | -725 | -420 | 994 | -218 | -854 | 767 | 349 | 651 |
| 152 | 848 | 356 | -1000 | 309 | 794 | -838 | -237 | 995 | -426 | -712 | 899 | 348 | 652 |
| 153 | 847 | 230 | -993 | 454 | 680 | -923 | -044 | 953 | -613 | -531 | 979 | 347 | 653 |
| 154 | 846 | 100 | -965 | 588 | 546 | -977 | 150 | 870 | -771 | -321 | 999 | 346 | 654 |
| 155 | 845 | -031 | -918 | 707 | 397 | -1000 | 339 | 750 | -891 | -094 | 960 | 345 | 655 |
| 156 | 844 | -163 | -851 | 809 | 237 | -989 | 514 | 598 | -969 | 138 | 864 | 344 | 656 |
| 157 | 843 | -291 | -767 | 891 | 069 | -945 | 671 | 420 | -1000 | 362 | 716 | 343 | 657 |
| 158 | 842 | -414 | -666 | 951 | -100 | -870 | 802 | 224 | -982 | 567 | 525 | 342 | 658 |
| 159 | 841 | -531 | -552 | 988 | -267 | -767 | 902 | 019 | -918 | 742 | 303 | 341 | 659 |
| 160 | 840 | -637 | -426 | 1000 | -426 | -637 | 969 | -187 | -809 | 876 | 063 | 340 | 660 |
| 161 | 839 | -733 | -291 | 988 | -572 | -487 | 998 | -386 | -661 | 964 | -181 | 339 | 661 |
| 162 | 838 | -816 | -150 | 951 | -703 | -321 | 990 | -567 | -482 | 999 | -414 | 338 | 662 |
| 163 | 837 | -885 | -006 | 891 | -813 | -144 | 945 | -725 | -279 | 981 | -623 | 337 | 663 |
| 164 | 836 | -939 | 138 | 809 | -899 | 038 | 864 | -851 | -063 | 910 | -794 | 336 | 664 |
| 165 | 835 | -976 | 279 | 707 | -960 | 218 | 750 | -941 | 156 | 790 | -918 | 335 | 665 |
| 166 | 834 | -996 | 414 | 588 | -994 | 391 | 608 | -990 | 368 | 628 | -987 | 334 | 666 |
| 167 | 833 | -999 | 541 | 454 | -998 | 552 | 443 | -998 | 562 | 431 | -997 | 333 | 667 |
| 168 | 832 | -985 | 657 | 309 | -975 | 694 | 261 | -962 | 729 | 212 | -947 | 332 | 668 |
| 169 | 831 | -953 | 758 | 156 | -923 | 813 | 069 | -885 | 861 | -019 | -841 | 331 | 669 |
| 170 | 830 | -905 | 844 | 000 | -844 | 905 | -125 | -771 | 951 | -249 | -685 | 330 | 670 |
| 171 | 829 | -841 | 913 | -156 | -742 | 967 | -315 | -623 | 996 | -465 | -487 | 329 | 671 |
| 172 | 828 | -762 | 962 | -309 | -618 | 997 | -493 | -448 | 992 | -657 | -261 | 328 | 672 |
| 173 | 827 | -671 | 991 | -454 | -476 | 994 | -652 | -255 | 941 | -813 | -019 | 327 | 673 |
| 174 | 826 | -567 | 1000 | -588 | -321 | 959 | -786 | -050 | 844 | -925 | 224 | 326 | 674 |
| 175 | 825 | -454 | 988 | -707 | -156 | 891 | -891 | 156 | 707 | -988 | 454 | 325 | 675 |
| 176 | 824 | -333 | 955 | -809 | 013 | 794 | -962 | 356 | 536 | -997 | 657 | 324 | 676 |
| 177 | 823 | -206 | 902 | -891 | 181 | 671 | -997 | 541 | 339 | -953 | 820 | 323 | 677 |
| 178 | 822 | -075 | 831 | -951 | 345 | 525 | -994 | 703 | 125 | -858 | 934 | 322 | 678 |
| 179 | 821 | 057 | 742 | -988 | 498 | 362 | -953 | 834 | -094 | -716 | 993 | 321 | 679 |

TABLE 8.5C (continued)
 $\cos 2\pi hx$ (h odd) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=1$ | 3 | 5 | 7 | 9 | 11 | 13 | 15 | 17 | 19 | Change sign.
x | |
|-----------------------|-----|-------|------|------|-------|------|------|-------|------|-------|-------|---------------------|-----|
| 180 | 820 | 426 | -969 | 809 | -063 | -729 | 992 | -536 | -309 | 930 | -876 | 320 | 680 |
| 181 | 819 | 420 | -964 | 827 | -107 | -689 | 998 | -603 | -218 | 885 | -927 | 319 | 681 |
| 182 | 818 | 414 | -959 | 844 | -150 | -647 | 1000 | -666 | -125 | 831 | -965 | 318 | 682 |
| 183 | 817 | 409 | -953 | 861 | -194 | -603 | 997 | -725 | -031 | 767 | -990 | 317 | 683 |
| 184 | 816 | 403 | -947 | 876 | -237 | -557 | 989 | -778 | 063 | 694 | -1000 | 316 | 684 |
| | | | | | | | | | | | | | |
| 185 | 815 | 397 | -941 | 891 | -279 | -509 | 976 | -827 | 156 | 613 | -996 | 315 | 685 |
| 186 | 814 | 391 | -934 | 905 | -321 | -460 | 959 | -870 | 249 | 525 | -977 | 314 | 686 |
| 187 | 813 | 386 | -927 | 918 | -362 | -409 | 937 | -907 | 339 | 431 | -945 | 313 | 687 |
| 188 | 812 | 380 | -920 | 930 | -403 | -356 | 910 | -939 | 426 | 333 | -899 | 312 | 688 |
| 189 | 811 | 374 | -913 | 941 | -443 | -303 | 879 | -964 | 509 | 230 | -841 | 311 | 689 |
| | | | | | | | | | | | | | |
| 190 | 810 | 368 | -905 | 951 | -482 | -249 | 844 | -982 | 588 | 125 | -771 | 310 | 690 |
| 191 | 809 | 362 | -897 | 960 | -520 | -194 | 805 | -994 | 661 | 019 | -689 | 309 | 691 |
| 192 | 808 | 356 | -888 | 969 | -557 | -138 | 762 | -1000 | 729 | -088 | -598 | 308 | 692 |
| 193 | 807 | 351 | -879 | 976 | -593 | -082 | 716 | -998 | 790 | -194 | -498 | 307 | 693 |
| 194 | 806 | 345 | -870 | 982 | -628 | -025 | 666 | -990 | 844 | -297 | -391 | 306 | 694 |
| | | | | | | | | | | | | | |
| 195 | 805 | 339 | -861 | 988 | -661 | 031 | 613 | -976 | 891 | -397 | -279 | 305 | 695 |
| 196 | 804 | 333 | -851 | 992 | -694 | 088 | 557 | -955 | 930 | -493 | -163 | 304 | 696 |
| 197 | 803 | 327 | -841 | 996 | -725 | 144 | 498 | -927 | 960 | -583 | -044 | 303 | 697 |
| 198 | 802 | 321 | -831 | 998 | -754 | 200 | 437 | -894 | 982 | -666 | 075 | 302 | 698 |
| 199 | 801 | 315 | -820 | 1000 | -782 | 255 | 374 | -854 | 996 | -742 | 194 | 301 | 699 |
| | | | | | | | | | | | | | |
| 200 | 800 | 309 | -809 | 1000 | -809 | 309 | 309 | -809 | 1000 | -809 | 309 | 300 | 700 |
| 201 | 789 | 303 | -798 | 1000 | -834 | 362 | 243 | -758 | 996 | -867 | 420 | 299 | 701 |
| 202 | 798 | 297 | -786 | 998 | -858 | 414 | 175 | -703 | 982 | -915 | 525 | 298 | 702 |
| 203 | 797 | 291 | -775 | 996 | -879 | 465 | 107 | -642 | 960 | -953 | 623 | 297 | 703 |
| 204 | 796 | 285 | -762 | 992 | -899 | 514 | 038 | -578 | 930 | -980 | 712 | 296 | 704 |
| | | | | | | | | | | | | | |
| 205 | 795 | 279 | -750 | 988 | -918 | 562 | -031 | -509 | 891 | -996 | 790 | 295 | 705 |
| 206 | 794 | 273 | -738 | 982 | -934 | 608 | -100 | -437 | 844 | -1000 | 858 | 294 | 706 |
| 207 | 793 | 267 | -725 | 976 | -949 | 652 | -169 | -362 | 790 | -993 | 913 | 293 | 707 |
| 208 | 792 | 261 | -712 | 969 | -962 | 694 | -237 | -285 | 729 | -975 | 955 | 292 | 708 |
| 209 | 791 | 255 | -698 | 960 | -973 | 733 | -303 | -206 | 661 | -945 | 983 | 291 | 709 |
| | | | | | | | | | | | | | |
| 210 | 790 | 249 | -685 | 951 | -982 | 771 | -368 | -125 | 588 | -905 | 998 | 290 | 710 |
| 211 | 789 | 243 | -671 | 941 | -990 | 805 | -431 | -044 | 509 | -854 | 998 | 289 | 711 |
| 212 | 788 | 237 | -657 | 930 | -995 | 838 | -493 | 038 | 426 | -794 | 985 | 288 | 712 |
| 213 | 787 | 230 | -642 | 918 | -998 | 867 | -552 | 119 | 339 | -725 | 957 | 287 | 713 |
| 214 | 786 | 224 | -628 | 905 | -1000 | 894 | -608 | 200 | 249 | -647 | 915 | 286 | 714 |
| | | | | | | | | | | | | | |
| 215 | 785 | 218 | -613 | 891 | -1000 | 918 | -661 | 279 | 156 | -562 | 861 | 285 | 715 |
| 216 | 784 | 212 | -598 | 876 | -997 | 939 | -712 | 356 | 063 | -471 | 794 | 284 | 716 |
| 217 | 783 | 206 | -583 | 861 | -993 | 957 | -758 | 431 | -031 | -374 | 716 | 283 | 717 |
| 218 | 782 | 200 | -567 | 844 | -987 | 972 | -802 | 504 | -125 | -273 | 628 | 282 | 718 |
| 219 | 781 | 194 | -552 | 827 | -979 | 983 | -841 | 572 | -218 | -169 | 531 | 281 | 719 |
| | | | | | | | | | | | | | |
| 220 | 780 | 187 | -536 | 809 | -969 | 992 | -876 | 637 | -309 | -063 | 426 | 280 | 720 |
| 221 | 779 | 181 | -520 | 790 | -957 | 998 | -907 | 698 | -397 | 044 | 315 | 279 | 721 |
| 222 | 778 | 175 | -504 | 771 | -943 | 1000 | -934 | 754 | -482 | 150 | 200 | 278 | 722 |
| 223 | 777 | 169 | -487 | 750 | -927 | 999 | -957 | 805 | -562 | 255 | 082 | 277 | 723 |
| 224 | 776 | 163 | -471 | 729 | -910 | 995 | -975 | 851 | -637 | 356 | -038 | 276 | 724 |

TABLE 8.5C (continued)

 $\cos 2\pi hx$ (h odd) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=21$ | 23 | 25 | 27 | 29 | 31 | 33 | 35 | 37 | 39 | Change sign.
x | |
|-----------------------|-----|--------|------|-------|------|-------|------|-------|------|------|-------|---------------------|-----|
| 180 | 820 | 187 | 637 | -1000 | 637 | 187 | -876 | 930 | -309 | -536 | 992 | 320 | 680 |
| 181 | 819 | 315 | 520 | -988 | 758 | 006 | -767 | 986 | -509 | -327 | 932 | 319 | 681 |
| 182 | 818 | 437 | 391 | -951 | 858 | -175 | -628 | 999 | -685 | -100 | 816 | 318 | 682 |
| 183 | 817 | 552 | 255 | -891 | 932 | -351 | -465 | 970 | -827 | 132 | 652 | 317 | 683 |
| 184 | 816 | 657 | 113 | -809 | 980 | -514 | -285 | 899 | -930 | 356 | 448 | 316 | 684 |
| 185 | 815 | 750 | -031 | -707 | 1000 | -661 | -094 | 790 | -988 | 562 | 218 | 315 | 685 |
| 186 | 814 | 831 | -175 | -588 | 990 | -786 | 100 | 647 | -998 | 737 | -025 | 314 | 686 |
| 187 | 813 | 897 | -315 | -454 | 953 | -885 | 291 | 476 | -960 | 873 | -267 | 313 | 687 |
| 188 | 812 | 947 | -448 | -309 | 888 | -955 | 471 | 285 | -876 | 962 | -493 | 312 | 688 |
| 189 | 811 | 981 | -572 | -156 | 798 | -993 | 633 | 082 | -750 | 999 | -689 | 311 | 689 |
| 190 | 810 | 998 | -685 | 000 | 685 | -998 | 771 | -125 | -588 | 982 | -844 | 310 | 690 |
| 191 | 809 | 998 | -782 | 156 | 552 | -970 | 879 | -327 | -397 | 913 | -949 | 309 | 691 |
| 192 | 808 | 980 | -864 | 309 | 403 | -910 | 955 | -514 | -187 | 794 | -997 | 308 | 692 |
| 193 | 807 | 945 | -927 | 454 | 243 | -820 | 994 | -680 | 031 | 633 | -986 | 307 | 693 |
| 194 | 806 | 894 | -972 | 588 | 075 | -703 | 996 | -816 | 249 | 437 | -915 | 306 | 694 |
| 195 | 805 | 827 | -996 | 707 | -094 | -562 | 960 | -918 | 454 | 218 | -790 | 305 | 695 |
| 196 | 804 | 746 | -999 | 809 | -261 | -403 | 888 | -980 | 637 | -013 | -618 | 304 | 696 |
| 197 | 803 | 652 | -981 | 891 | -420 | -230 | 782 | -1000 | 790 | -243 | -409 | 303 | 697 |
| 198 | 802 | 546 | -943 | 951 | -567 | -050 | 647 | -977 | 905 | -460 | -175 | 302 | 698 |
| 199 | 801 | 431 | -885 | 988 | -698 | 132 | 487 | -913 | 976 | -652 | 069 | 301 | 699 |
| 200 | 800 | 309 | -809 | 1000 | -809 | 309 | 309 | -809 | 1000 | -809 | 309 | 300 | 700 |
| 201 | 799 | 181 | -716 | 988 | -897 | 476 | 119 | -671 | 976 | -923 | 531 | 299 | 701 |
| 202 | 798 | 050 | -608 | 951 | -959 | 628 | -075 | -504 | 905 | -987 | 720 | 298 | 702 |
| 203 | 797 | -082 | -487 | 891 | -993 | 758 | -267 | -315 | 790 | -998 | 867 | 297 | 703 |
| 204 | 796 | -212 | -356 | 809 | -999 | 864 | -448 | -113 | 637 | -955 | 962 | 296 | 704 |
| 205 | 795 | -339 | -218 | 707 | -976 | 941 | -613 | 094 | 454 | -861 | 1000 | 295 | 705 |
| 206 | 794 | -460 | -075 | 588 | -925 | 987 | -754 | 297 | 249 | -720 | 977 | 294 | 706 |
| 207 | 793 | -572 | 069 | 454 | -848 | 1000 | -867 | 487 | 031 | -541 | 897 | 293 | 707 |
| 208 | 792 | -675 | 212 | 309 | -746 | 980 | -947 | 657 | -187 | -333 | 762 | 292 | 708 |
| 209 | 791 | -767 | 351 | 156 | -623 | 927 | -991 | 798 | -397 | -107 | 583 | 291 | 709 |
| 210 | 790 | -844 | 482 | 000 | -482 | 844 | -998 | 905 | -588 | 125 | 368 | 290 | 710 |
| 211 | 789 | -907 | 603 | -156 | -327 | 733 | -967 | 973 | -750 | 351 | 132 | 289 | 711 |
| 212 | 788 | -955 | 712 | -309 | -163 | 598 | -899 | 1000 | -876 | 557 | -113 | 288 | 712 |
| 213 | 787 | -986 | 805 | -454 | 006 | 443 | -798 | 983 | -960 | 733 | -351 | 287 | 713 |
| 214 | 786 | -999 | 882 | -588 | 175 | 273 | -666 | 925 | -998 | 870 | -567 | 286 | 714 |
| 215 | 785 | -996 | 941 | -707 | 339 | 094 | -509 | 827 | -988 | 960 | -750 | 285 | 715 |
| 216 | 784 | -975 | 980 | -809 | 493 | -088 | -333 | 694 | -930 | 999 | -888 | 284 | 716 |
| 217 | 783 | -937 | 998 | -891 | 633 | -267 | -144 | 531 | -827 | 983 | -973 | 283 | 717 |
| 218 | 782 | -882 | 996 | -951 | 754 | -437 | 050 | 345 | -685 | 915 | -1000 | 282 | 718 |
| 219 | 781 | -813 | 973 | -988 | 854 | -593 | 243 | 144 | -509 | 798 | -967 | 281 | 719 |
| 220 | 780 | -729 | 930 | -1000 | 930 | -729 | 426 | -063 | -309 | 637 | -876 | 280 | 720 |
| 221 | 779 | -633 | 867 | -988 | 979 | -841 | 593 | -267 | -094 | 443 | -733 | 279 | 721 |
| 222 | 778 | -525 | 786 | -951 | 999 | -925 | 737 | -460 | 125 | 224 | -546 | 278 | 722 |
| 223 | 777 | -409 | 689 | -891 | 991 | -979 | 854 | -633 | 339 | -006 | -327 | 277 | 723 |
| 224 | 776 | -285 | 578 | -809 | 955 | -1000 | 939 | -778 | 536 | -237 | -088 | 276 | 724 |

TABLE 8.5C (*continued*)
 $\cos 2\pi hx$ (h odd) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=1$ | 3 | 5 | 7 | 9 | 11 | 13 | 15 | 17 | 19 | Change sign.
x | |
|-----------------------|-----|-------|------|-----|------|-----|-------|------|-------|------|-------|---------------------|-----|
| 225 | 775 | 156 | -454 | 707 | -891 | 988 | -988 | 891 | -707 | 454 | -156 | 275 | 725 |
| 226 | 774 | 150 | -437 | 685 | -870 | 977 | -996 | 925 | -771 | 546 | -273 | 274 | 726 |
| 227 | 773 | 144 | -420 | 661 | -848 | 964 | -1000 | 953 | -827 | 633 | -386 | 273 | 727 |
| 228 | 772 | 138 | -403 | 637 | -824 | 947 | -999 | 975 | -876 | 712 | -493 | 272 | 728 |
| 229 | 771 | 132 | -386 | 613 | -798 | 927 | -993 | 990 | -918 | 782 | -593 | 271 | 729 |
| | | | | | | | | | | | | | |
| 230 | 770 | 125 | -368 | 588 | -771 | 905 | -982 | 998 | -951 | 844 | -685 | 270 | 730 |
| 231 | 769 | 119 | -351 | 562 | -742 | 879 | -967 | 1000 | -976 | 897 | -767 | 269 | 731 |
| 232 | 768 | 113 | -333 | 536 | -712 | 851 | -947 | 995 | -992 | 939 | -838 | 268 | 732 |
| 233 | 767 | 107 | -315 | 509 | -680 | 820 | -923 | 983 | -1000 | 970 | -897 | 267 | 733 |
| 234 | 766 | 100 | -297 | 482 | -647 | 786 | -894 | 965 | -998 | 990 | -943 | 266 | 734 |
| | | | | | | | | | | | | | |
| 235 | 765 | 094 | -279 | 454 | -613 | 750 | -861 | 941 | -988 | 1000 | -976 | 265 | 735 |
| 236 | 764 | 088 | -261 | 426 | -578 | 712 | -824 | 910 | -969 | 997 | -995 | 264 | 736 |
| 237 | 763 | 082 | -243 | 397 | -541 | 671 | -782 | 873 | -941 | 983 | -1000 | 263 | 737 |
| 238 | 762 | 075 | -224 | 368 | -504 | 628 | -738 | 831 | -905 | 959 | -990 | 262 | 738 |
| 239 | 761 | 069 | -206 | 339 | -465 | 583 | -689 | 782 | -861 | 923 | -967 | 261 | 739 |
| | | | | | | | | | | | | | |
| 240 | 760 | 063 | -187 | 309 | -426 | 536 | -637 | 729 | -809 | 876 | -930 | 260 | 740 |
| 241 | 759 | 057 | -169 | 279 | -386 | 487 | -583 | 671 | -750 | 820 | -879 | 259 | 741 |
| 242 | 758 | 050 | -150 | 249 | -345 | 437 | -525 | 608 | -685 | 754 | -816 | 258 | 742 |
| 243 | 757 | 044 | -132 | 218 | -303 | 386 | -465 | 541 | -613 | 680 | -742 | 257 | 743 |
| 244 | 756 | 038 | -113 | 187 | -261 | 333 | -403 | 471 | -536 | 598 | -657 | 256 | 744 |
| | | | | | | | | | | | | | |
| 245 | 755 | 031 | -094 | 156 | -218 | 279 | -339 | 397 | -454 | 509 | -562 | 255 | 745 |
| 246 | 754 | 025 | -075 | 125 | -175 | 224 | -273 | 321 | -368 | 414 | -460 | 254 | 746 |
| 247 | 753 | 019 | -057 | 094 | -132 | 169 | -206 | 243 | -279 | 315 | -351 | 253 | 747 |
| 248 | 752 | 013 | -038 | 063 | -088 | 113 | -138 | 163 | -187 | 212 | -237 | 252 | 748 |
| 249 | 751 | 006 | -019 | 031 | -044 | 057 | -069 | 082 | -094 | 107 | -119 | 251 | 749 |
| | | | | | | | | | | | | | |
| 250 | 750 | 000 | 000 | 000 | 000 | 000 | 000 | 000 | 000 | 000 | 000 | 250 | 750 |

TABLE 8.5C (continued)

 $\cos 2\pi hx$ (h odd) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=21$ | 23 | 25 | 27 | 29 | 31 | 33 | 35 | 37 | 39 | Change sign.
x | |
|-----------------------|-----|--------|-------|------|------|------|-------|------|-------|------|------|---------------------|-----|
| 225 | 775 | -156 | 454 | -707 | 891 | -988 | 988 | -891 | 707 | -454 | 156 | 275 | 725 |
| 226 | 774 | -025 | 321 | -588 | 802 | -943 | 999 | -965 | 844 | -647 | 391 | 274 | 726 |
| 227 | 773 | 107 | 181 | -454 | 689 | -867 | 973 | -998 | 941 | -805 | 603 | 273 | 727 |
| 228 | 772 | 237 | 038 | -309 | 557 | -762 | 910 | -989 | 992 | -920 | 778 | 272 | 728 |
| 229 | 771 | 362 | -107 | -156 | 409 | -633 | 813 | -937 | 996 | -986 | 907 | 271 | 729 |
| | | | | | | | | | | | | | |
| 230 | 770 | 482 | -249 | 000 | 249 | -482 | 685 | -844 | 951 | -998 | 982 | 270 | 730 |
| 231 | 769 | 593 | -386 | 156 | 082 | -315 | 531 | -716 | 861 | -957 | 998 | 269 | 731 |
| 232 | 768 | 694 | -514 | 309 | -088 | -138 | 356 | -557 | 729 | -864 | 955 | 268 | 732 |
| 233 | 767 | 782 | -633 | 454 | -255 | 044 | 169 | -374 | 562 | -725 | 854 | 267 | 733 |
| 234 | 766 | 858 | -738 | 588 | -414 | 224 | -025 | -175 | 368 | -546 | 703 | 266 | 734 |
| | | | | | | | | | | | | | |
| 235 | 765 | 918 | -827 | 707 | -562 | 397 | -218 | 031 | 156 | -339 | 509 | 265 | 735 |
| 236 | 764 | 962 | -899 | 809 | -694 | 557 | -403 | 237 | -063 | -113 | 285 | 264 | 736 |
| 237 | 763 | 990 | -953 | 891 | -805 | 698 | -572 | 431 | -279 | 119 | 044 | 263 | 737 |
| 238 | 762 | 1000 | -987 | 951 | -894 | 816 | -720 | 608 | -482 | 345 | -200 | 262 | 738 |
| 239 | 761 | 993 | -1000 | 988 | -957 | 907 | -841 | 758 | -661 | 552 | -431 | 261 | 739 |
| | | | | | | | | | | | | | |
| 240 | 760 | 969 | -992 | 1000 | -992 | 969 | -930 | 876 | -809 | 729 | -637 | 260 | 740 |
| 241 | 759 | 927 | -964 | 988 | -999 | 998 | -983 | 957 | -918 | 867 | -805 | 259 | 741 |
| 242 | 758 | 870 | -915 | 951 | -977 | 994 | -1000 | 996 | -982 | 959 | -925 | 258 | 742 |
| 243 | 757 | 798 | -848 | 891 | -927 | 957 | -979 | 993 | -1000 | 998 | -990 | 257 | 743 |
| 244 | 756 | 712 | -762 | 809 | -851 | 888 | -920 | 947 | -969 | 985 | -995 | 256 | 744 |
| | | | | | | | | | | | | | |
| 245 | 755 | 613 | -661 | 707 | -750 | 790 | -827 | 861 | -891 | 918 | -941 | 255 | 745 |
| 246 | 754 | 504 | -546 | 588 | -628 | 666 | -703 | 738 | -771 | 802 | -831 | 254 | 746 |
| 247 | 753 | 386 | -420 | 454 | -487 | 520 | -552 | 583 | -613 | 642 | -671 | 253 | 747 |
| 248 | 752 | 261 | -285 | 309 | -333 | 356 | -380 | 403 | -426 | 448 | -471 | 252 | 748 |
| 249 | 751 | 132 | -144 | 156 | -169 | 181 | -194 | 206 | -218 | 230 | -243 | 251 | 749 |
| | | | | | | | | | | | | | |
| 250 | 750 | 000 | 000 | 000 | 000 | 000 | 000 | 000 | 000 | 000 | 000 | 250 | 750 |

TABLE 8.5D

 $\cos 2\pi hx$ (h even) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=2$ | 4 | 6 | 8 | 10 | 12 | 14 | 16 | 18 | 20 | Change sign for $h=4n+2$
Sign as given for $h=4n$
x | |
|-----------------------|-----|-------|------|------|------|------|-------|-------|-------|-------|-------|---|-----|
| 000 | 500 | 1000 | 1000 | 1000 | 1000 | 1000 | 1000 | 1000 | 1000 | 1000 | 1000 | 250 | 750 |
| 001 | 501 | 1000 | 1000 | 999 | 999 | 998 | 997 | 996 | 995 | 994 | 992 | 251 | 751 |
| 002 | 502 | 1000 | 999 | 997 | 995 | 992 | 989 | 985 | 980 | 975 | 969 | 252 | 752 |
| 003 | 503 | 999 | 997 | 994 | 989 | 982 | 975 | 965 | 955 | 943 | 930 | 253 | 753 |
| 004 | 504 | 999 | 995 | 989 | 980 | 969 | 955 | 939 | 920 | 899 | 876 | 254 | 754 |
| | | | | | | | | | | | | | |
| 005 | 505 | 998 | 992 | 982 | 969 | 951 | 930 | 905 | 876 | 844 | 809 | 255 | 755 |
| 006 | 506 | 997 | 989 | 975 | 955 | 930 | 899 | 864 | 824 | 778 | 729 | 256 | 756 |
| 007 | 507 | 996 | 985 | 965 | 939 | 905 | 864 | 816 | 762 | 703 | 637 | 257 | 757 |
| 008 | 508 | 995 | 980 | 955 | 920 | 876 | 824 | 762 | 694 | 618 | 536 | 258 | 758 |
| 009 | 509 | 994 | 975 | 943 | 899 | 844 | 778 | 703 | 618 | 525 | 426 | 259 | 759 |
| | | | | | | | | | | | | | |
| 010 | 510 | 992 | 969 | 930 | 876 | 809 | 729 | 637 | 536 | 426 | 309 | 260 | 760 |
| 011 | 511 | 990 | 962 | 915 | 851 | 771 | 675 | 567 | 448 | 321 | 187 | 261 | 761 |
| 012 | 512 | 989 | 955 | 899 | 824 | 729 | 618 | 493 | 356 | 212 | 063 | 262 | 762 |
| 013 | 513 | 987 | 947 | 882 | 794 | 685 | 557 | 414 | 261 | 100 | -063 | 263 | 763 |
| 014 | 514 | 985 | 939 | 864 | 762 | 637 | 493 | 333 | 163 | -013 | -187 | 264 | 764 |
| | | | | | | | | | | | | | |
| 015 | 515 | 982 | 930 | 844 | 729 | 588 | 426 | 249 | 063 | -125 | -309 | 265 | 765 |
| 016 | 516 | 980 | 920 | 824 | 694 | 536 | 356 | 163 | -038 | -237 | -426 | 266 | 766 |
| 017 | 517 | 977 | 910 | 802 | 657 | 482 | 285 | 075 | -138 | -345 | -536 | 267 | 767 |
| 018 | 518 | 975 | 899 | 778 | 618 | 426 | 212 | -013 | -237 | -448 | -637 | 268 | 768 |
| 019 | 519 | 972 | 888 | 754 | 578 | 368 | 138 | -100 | -333 | -546 | -729 | 269 | 769 |
| | | | | | | | | | | | | | |
| 020 | 520 | 969 | 876 | 729 | 536 | 309 | 063 | -187 | -426 | -637 | -809 | 270 | 770 |
| 021 | 521 | 965 | 864 | 703 | 493 | 249 | -013 | -273 | -514 | -720 | -876 | 271 | 771 |
| 022 | 522 | 962 | 851 | 675 | 448 | 187 | -088 | -356 | -598 | -794 | -930 | 272 | 772 |
| 023 | 523 | 959 | 838 | 647 | 403 | 125 | -163 | -437 | -675 | -858 | -969 | 273 | 773 |
| 024 | 524 | 955 | 824 | 618 | 356 | 063 | -237 | -514 | -746 | -910 | -992 | 274 | 774 |
| | | | | | | | | | | | | | |
| 025 | 525 | 951 | 809 | 588 | 309 | 000 | -309 | -588 | -809 | -951 | -1000 | 275 | 775 |
| 026 | 526 | 947 | 794 | 557 | 261 | -063 | -380 | -657 | -864 | -980 | -992 | 276 | 776 |
| 027 | 527 | 943 | 778 | 525 | 212 | -125 | -448 | -720 | -910 | -996 | -969 | 277 | 777 |
| 028 | 528 | 939 | 762 | 493 | 163 | -187 | -514 | -778 | -947 | -1000 | -930 | 278 | 778 |
| 029 | 529 | 934 | 746 | 460 | 113 | -249 | -578 | -831 | -975 | -990 | -876 | 279 | 779 |
| | | | | | | | | | | | | | |
| 030 | 530 | 930 | 729 | 426 | 063 | -309 | -637 | -876 | -992 | -969 | -809 | 280 | 780 |
| 031 | 531 | 925 | 712 | 391 | 013 | -368 | -694 | -915 | -1000 | -934 | -729 | 281 | 781 |
| 032 | 532 | 920 | 694 | 356 | -038 | -426 | -746 | -947 | -997 | -888 | -637 | 282 | 782 |
| 033 | 533 | 915 | 675 | 321 | -088 | -482 | -794 | -972 | -985 | -831 | -536 | 283 | 783 |
| 034 | 534 | 910 | 657 | 285 | -138 | -536 | -838 | -989 | -962 | -762 | -426 | 284 | 784 |
| | | | | | | | | | | | | | |
| 035 | 535 | 905 | 637 | 249 | -187 | -588 | -876 | -998 | -930 | -685 | -309 | 285 | 785 |
| 036 | 536 | 899 | 618 | 212 | -237 | -637 | -910 | -1000 | -888 | -598 | -187 | 286 | 786 |
| 037 | 537 | 894 | 598 | 175 | -285 | -685 | -939 | -994 | -838 | -504 | -063 | 287 | 787 |
| 038 | 538 | 888 | 578 | 138 | -333 | -729 | -962 | -980 | -778 | -403 | 063 | 288 | 788 |
| 039 | 539 | 882 | 557 | 100 | -380 | -771 | -980 | -959 | -712 | -297 | 187 | 289 | 789 |
| | | | | | | | | | | | | | |
| 040 | 540 | 876 | 536 | 063 | -426 | -809 | -992 | -930 | -637 | -187 | 309 | 290 | 790 |
| 041 | 541 | 870 | 514 | 025 | -471 | -844 | -999 | -894 | -557 | -075 | 426 | 291 | 791 |
| 042 | 542 | 864 | 493 | -013 | -514 | -876 | -1000 | -851 | -471 | 038 | 536 | 292 | 792 |
| 043 | 543 | 858 | 471 | -050 | -557 | -905 | -995 | -802 | -380 | 150 | 637 | 293 | 793 |
| 044 | 544 | 851 | 448 | -088 | -598 | -930 | -985 | -746 | -285 | 261 | 729 | 294 | 794 |

TABLE 8.5D

 $\cos 2\pi hx$ (h even) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=22$ | 24 | 26 | 28 | 30 | 32 | 34 | 36 | 38 | 40 | Change sign for $h=4n+2$
Sign as given for $h=4n$
x | |
|-----------------------|-----|--------|-------|------|-------|------|------|-------|-------|------|------|---|-----|
| 000 | 500 | 1000 | 1000 | 1000 | 1000 | 1000 | 1000 | 1000 | 1000 | 1000 | 1000 | 250 | 750 |
| 001 | 501 | 990 | 989 | 987 | 985 | 982 | 980 | 977 | 975 | 972 | 969 | 251 | 751 |
| 002 | 502 | 962 | 955 | 947 | 939 | 930 | 920 | 910 | 899 | 888 | 876 | 252 | 752 |
| 003 | 503 | 915 | 899 | 882 | 864 | 844 | 824 | 802 | 778 | 754 | 729 | 253 | 753 |
| 004 | 504 | 851 | 824 | 794 | 762 | 729 | 694 | 657 | 618 | 578 | 536 | 254 | 754 |
| 005 | 505 | 771 | 729 | 685 | 637 | 588 | 536 | 482 | 426 | 368 | 309 | 255 | 755 |
| 006 | 506 | 675 | 618 | 557 | 493 | 426 | 356 | 285 | 212 | 138 | 063 | 256 | 756 |
| 007 | 507 | 567 | 493 | 414 | 333 | 249 | 163 | 075 | -013 | -100 | -187 | 257 | 757 |
| 008 | 508 | 448 | 356 | 261 | 163 | 063 | -038 | -138 | -237 | -333 | -426 | 258 | 758 |
| 009 | 509 | 321 | 212 | 100 | -013 | -125 | -237 | -345 | -448 | -546 | -637 | 259 | 759 |
| 010 | 510 | 187 | 063 | -063 | -187 | -309 | -426 | -536 | -637 | -729 | -809 | 260 | 760 |
| 011 | 511 | 050 | -088 | -224 | -356 | -482 | -598 | -703 | -794 | -870 | -930 | 261 | 761 |
| 012 | 512 | -088 | -237 | -380 | -514 | -637 | -746 | -838 | -910 | -962 | -992 | 262 | 762 |
| 013 | 513 | -224 | -380 | -525 | -657 | -771 | -864 | -934 | -980 | -999 | -992 | 263 | 763 |
| 014 | 514 | -356 | -514 | -657 | -778 | -876 | -947 | -989 | -1000 | -980 | -930 | 264 | 764 |
| 015 | 515 | -482 | -637 | -771 | -876 | -951 | -992 | -998 | -969 | -905 | -809 | 265 | 765 |
| 016 | 516 | -598 | -746 | -864 | -947 | -992 | -997 | -962 | -888 | -778 | -637 | 266 | 766 |
| 017 | 517 | -703 | -838 | -934 | -989 | -998 | -962 | -882 | -762 | -608 | -426 | 267 | 767 |
| 018 | 518 | -794 | -910 | -980 | -1000 | -969 | -888 | -762 | -598 | -403 | -187 | 268 | 768 |
| 019 | 519 | -870 | -962 | -999 | -980 | -905 | -778 | -608 | -403 | -175 | 063 | 269 | 769 |
| 020 | 520 | -930 | -992 | -992 | -930 | -809 | -637 | -426 | -187 | 063 | 309 | 270 | 770 |
| 021 | 521 | -972 | -1000 | -959 | -851 | -685 | -471 | -224 | 038 | 297 | 536 | 271 | 771 |
| 022 | 522 | -995 | -985 | -899 | -746 | -536 | -285 | -013 | 261 | 514 | 729 | 272 | 772 |
| 023 | 523 | -999 | -947 | -816 | -618 | -368 | -088 | 200 | 471 | 703 | 876 | 273 | 773 |
| 024 | 524 | -985 | -888 | -712 | -471 | -187 | 113 | 403 | 657 | 851 | 969 | 274 | 774 |
| 025 | 525 | -951 | -809 | -588 | -309 | 000 | 309 | 588 | 809 | 951 | 1000 | 275 | 775 |
| 026 | 526 | -899 | -712 | -448 | -138 | 187 | 493 | 746 | 920 | 997 | 969 | 276 | 776 |
| 027 | 527 | -831 | -598 | -297 | 038 | 368 | 657 | 870 | 985 | 987 | 876 | 277 | 777 |
| 028 | 528 | -746 | -471 | -138 | 212 | 536 | 794 | 955 | 999 | 920 | 729 | 278 | 778 |
| 029 | 529 | -647 | -333 | 025 | 380 | 685 | 899 | 996 | 962 | 802 | 536 | 279 | 779 |
| 030 | 530 | -536 | -187 | 187 | 536 | 809 | 969 | 992 | 876 | 637 | 309 | 280 | 780 |
| 031 | 531 | -414 | -038 | 345 | 675 | 905 | 999 | 943 | 746 | 437 | 063 | 281 | 781 |
| 032 | 532 | -285 | 113 | 493 | 794 | 969 | 989 | 851 | 578 | 212 | -187 | 282 | 782 |
| 033 | 533 | -150 | 261 | 628 | 888 | 998 | 939 | 720 | 380 | -025 | -426 | 283 | 783 |
| 034 | 534 | -013 | 403 | 746 | 955 | 992 | 851 | 557 | 163 | -261 | -637 | 284 | 784 |
| 035 | 535 | 125 | 536 | 844 | 992 | 951 | 729 | 368 | -063 | -482 | -809 | 285 | 785 |
| 036 | 536 | 261 | 657 | 920 | 999 | 876 | 578 | 163 | -285 | -675 | -930 | 286 | 786 |
| 037 | 537 | 391 | 762 | 972 | 975 | 771 | 403 | -050 | -493 | -831 | -992 | 287 | 787 |
| 038 | 538 | 514 | 851 | 997 | 920 | 637 | 212 | -261 | -675 | -939 | -992 | 288 | 788 |
| 039 | 539 | 628 | 920 | 996 | 838 | 482 | 013 | -460 | -824 | -994 | -930 | 289 | 789 |
| 040 | 540 | 729 | 969 | 969 | 729 | 309 | -187 | -637 | -930 | -992 | -809 | 290 | 790 |
| 041 | 541 | 816 | 995 | 915 | 598 | 125 | -380 | -786 | -989 | -934 | -637 | 291 | 791 |
| 042 | 542 | 888 | 999 | 838 | 448 | -063 | -557 | -899 | -997 | -824 | -426 | 292 | 792 |
| 043 | 543 | 943 | 980 | 738 | 285 | -249 | -712 | -972 | -955 | -666 | -187 | 293 | 793 |
| 044 | 544 | 980 | 939 | 618 | 113 | -426 | -838 | -1000 | -864 | -471 | 063 | 294 | 794 |

TABLE 8.5D (continued)

 $\cos 2\pi hx$ (h even) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=2$ | 4 | 6 | 8 | 10 | 12 | 14 | 16 | 18 | 20 | Change sign for $h=4n+2$
Sign as given for $h=4n$
x | |
|-----------------------|-----|-------|------|-------|-------|-------|------|------|------|------|-------|---|-----|
| 045 | 545 | 844 | 426 | -125 | -637 | -951 | -969 | -685 | -187 | 368 | 809 | 295 | 795 |
| 046 | 546 | 838 | 403 | -163 | -675 | -969 | -947 | -618 | -088 | 471 | 876 | 296 | 796 |
| 047 | 547 | 831 | 380 | -200 | -712 | -982 | -920 | -546 | 013 | 567 | 930 | 297 | 797 |
| 048 | 548 | 824 | 356 | -237 | -746 | -992 | -888 | -471 | 113 | 657 | 969 | 298 | 798 |
| 049 | 549 | 816 | 333 | -273 | -778 | -998 | -851 | -391 | 212 | 737 | 992 | 299 | 799 |
| 050 | 550 | 809 | 309 | -309 | -809 | -1000 | -809 | -309 | 309 | 809 | 1000 | 300 | 800 |
| 051 | 551 | 802 | 285 | -345 | -838 | -998 | -762 | -224 | 403 | 870 | 992 | 301 | 801 |
| 052 | 552 | 794 | 261 | -380 | -864 | -992 | -712 | -138 | 493 | 920 | 969 | 302 | 802 |
| 053 | 553 | 786 | 237 | -414 | -888 | -982 | -657 | -050 | 578 | 959 | 930 | 303 | 803 |
| 054 | 554 | 778 | 212 | -448 | -910 | -969 | -598 | 038 | 657 | 985 | 876 | 304 | 804 |
| 055 | 555 | 771 | 187 | -482 | -930 | -951 | -536 | 125 | 729 | 998 | 809 | 305 | 805 |
| 056 | 556 | 762 | 163 | -514 | -947 | -930 | -471 | 212 | 794 | 999 | 729 | 306 | 806 |
| 057 | 557 | 754 | 138 | -546 | -962 | -905 | -403 | 297 | 851 | 987 | 637 | 307 | 807 |
| 058 | 558 | 746 | 113 | -578 | -975 | -876 | -333 | 380 | 899 | 962 | 536 | 308 | 808 |
| 059 | 559 | 738 | 088 | -608 | -985 | -844 | -261 | 460 | 939 | 925 | 426 | 309 | 809 |
| 060 | 560 | 729 | 063 | -637 | -992 | -809 | -187 | 536 | 969 | 876 | 309 | 310 | 810 |
| 061 | 561 | 720 | 038 | -666 | -997 | -771 | -113 | 608 | 989 | 816 | 187 | 311 | 811 |
| 062 | 562 | 712 | 013 | -694 | -1000 | -729 | -038 | 675 | 999 | 746 | 063 | 312 | 812 |
| 063 | 563 | 703 | -013 | -720 | -1000 | -685 | 038 | 737 | 999 | 666 | -063 | 313 | 813 |
| 064 | 564 | 694 | -038 | -746 | -997 | -637 | 113 | 794 | 989 | 578 | -187 | 314 | 814 |
| 065 | 565 | 685 | -063 | -771 | -992 | -588 | 187 | 844 | 969 | 482 | -309 | 315 | 815 |
| 066 | 566 | 675 | -088 | -794 | -985 | -536 | 261 | 888 | 939 | 380 | -426 | 316 | 816 |
| 067 | 567 | 666 | -113 | -816 | -975 | -482 | 333 | 925 | 899 | 273 | -536 | 317 | 817 |
| 068 | 568 | 657 | -138 | -838 | -962 | -426 | 403 | 955 | 851 | 163 | -637 | 318 | 818 |
| 069 | 569 | 647 | -163 | -858 | -947 | -368 | 471 | 977 | 794 | 050 | -729 | 319 | 819 |
| 070 | 570 | 637 | -187 | -876 | -930 | -309 | 536 | 992 | 729 | -063 | -809 | 320 | 820 |
| 071 | 571 | 628 | -212 | -894 | -910 | -249 | 598 | 999 | 657 | -175 | -876 | 321 | 821 |
| 072 | 572 | 618 | -237 | -910 | -888 | -187 | 657 | 999 | 578 | -285 | -930 | 322 | 822 |
| 073 | 573 | 608 | -261 | -925 | -864 | -125 | 712 | 990 | 493 | -391 | -969 | 323 | 823 |
| 074 | 574 | 598 | -285 | -939 | -838 | -063 | 762 | 975 | 403 | -493 | -992 | 324 | 824 |
| 075 | 575 | 588 | -309 | -951 | -809 | 000 | 809 | 951 | 309 | -588 | -1000 | 325 | 825 |
| 076 | 576 | 578 | -333 | -962 | -778 | 063 | 851 | 920 | 212 | -675 | -992 | 326 | 826 |
| 077 | 577 | 567 | -356 | -972 | -746 | 125 | 888 | 882 | 113 | -754 | -969 | 327 | 827 |
| 078 | 578 | 557 | -380 | -980 | -712 | 187 | 920 | 838 | 013 | -824 | -930 | 328 | 828 |
| 079 | 579 | 546 | -403 | -987 | -675 | 249 | 947 | 786 | -088 | -882 | -876 | 329 | 829 |
| 080 | 580 | 536 | -426 | -992 | -637 | 309 | 969 | 729 | -187 | -930 | -809 | 330 | 830 |
| 081 | 581 | 525 | -448 | -996 | -598 | 368 | 985 | 666 | -285 | -965 | -729 | 331 | 831 |
| 082 | 582 | 514 | -471 | -999 | -557 | 426 | 995 | 598 | -380 | -989 | -637 | 332 | 832 |
| 083 | 583 | 504 | -493 | -1000 | -514 | 482 | 1000 | 525 | -471 | -999 | -536 | 333 | 833 |
| 084 | 584 | 493 | -514 | -1000 | -471 | 536 | 999 | 448 | -557 | -997 | -426 | 334 | 834 |
| 085 | 585 | 482 | -536 | -998 | -426 | 588 | 992 | 368 | -637 | -982 | -309 | 335 | 835 |
| 086 | 586 | 471 | -557 | -995 | -380 | 637 | 980 | 285 | -712 | -955 | -187 | 336 | 836 |
| 087 | 587 | 460 | -578 | -990 | -333 | 685 | 962 | 200 | -778 | -915 | -063 | 337 | 837 |
| 088 | 588 | 448 | -598 | -985 | -285 | 729 | 939 | 113 | -838 | -864 | 063 | 338 | 838 |
| 089 | 589 | 437 | -618 | -977 | -237 | 771 | 910 | 025 | -888 | -802 | 187 | 339 | 839 |

TABLE 8.5D (continued)

 $\cos 2\pi hx$ (h even) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=22$ | 24 | 26 | 28 | 30 | 32 | 34 | 36 | 38 | 40 | Change sign for $h=4n+2$
Sign as given for $h=4n$
x | |
|-----------------------|-----|--------|------|------|------|-------|-------|------|------|------|------|---|-----|
| 045 | 545 | 998 | 876 | 482 | -063 | -588 | -930 | -982 | -729 | -249 | 309 | 295 | 795 |
| 046 | 546 | 997 | 794 | 333 | -237 | -729 | -985 | -920 | -557 | -013 | 536 | 296 | 796 |
| 047 | 547 | 977 | 694 | 175 | -403 | -844 | -1000 | -816 | -356 | 224 | 729 | 297 | 797 |
| 048 | 548 | 939 | 578 | 013 | -557 | -930 | -975 | -675 | -138 | 448 | 876 | 298 | 798 |
| 049 | 549 | 882 | 448 | -150 | -694 | -982 | -910 | -504 | 088 | 647 | 969 | 299 | 799 |
| 050 | 550 | 809 | 309 | -309 | -809 | -1000 | -809 | -309 | 309 | 809 | 1000 | 300 | 800 |
| 051 | 551 | 720 | 163 | -460 | -899 | -982 | -675 | -100 | 514 | 925 | 969 | 301 | 801 |
| 052 | 552 | 618 | 013 | -598 | -962 | -930 | -514 | 113 | 694 | 989 | 876 | 302 | 802 |
| 053 | 553 | 504 | -138 | -720 | -995 | -844 | -333 | 321 | 838 | 996 | 729 | 303 | 803 |
| 054 | 554 | 380 | -285 | -824 | -997 | -729 | -138 | 514 | 939 | 947 | 536 | 304 | 804 |
| 055 | 555 | 249 | -426 | -905 | -969 | -588 | 063 | 685 | 992 | 844 | 309 | 305 | 805 |
| 056 | 556 | 113 | -557 | -962 | -910 | -426 | 261 | 824 | 995 | 694 | 063 | 306 | 806 |
| 057 | 557 | -025 | -675 | -994 | -824 | -249 | 448 | 925 | 947 | 504 | -187 | 307 | 807 |
| 058 | 558 | -163 | -778 | -999 | -712 | -063 | 618 | 985 | 851 | 285 | -426 | 308 | 808 |
| 059 | 559 | -297 | -864 | -977 | -578 | 125 | 762 | 999 | 712 | 050 | -637 | 309 | 809 |
| 060 | 560 | -426 | -930 | -930 | -426 | 309 | 876 | 969 | 536 | -187 | -809 | 310 | 810 |
| 061 | 561 | -546 | -975 | -858 | -261 | 482 | 955 | 894 | 333 | -414 | -930 | 311 | 811 |
| 062 | 562 | -657 | -997 | -762 | -088 | 637 | 995 | 778 | 113 | -618 | -992 | 312 | 812 |
| 063 | 563 | -754 | -997 | -647 | 088 | 771 | 995 | 628 | -113 | -786 | -992 | 313 | 813 |
| 064 | 564 | -838 | -975 | -514 | 261 | 876 | 955 | 448 | -333 | -910 | -930 | 314 | 814 |
| 065 | 565 | -905 | -930 | -368 | 426 | 951 | 876 | 249 | -536 | -982 | -809 | 315 | 815 |
| 066 | 566 | -955 | -864 | -212 | 578 | 992 | 762 | 038 | -712 | -999 | -637 | 316 | 816 |
| 067 | 567 | -987 | -778 | -050 | 712 | 998 | 618 | -175 | -851 | -959 | -426 | 317 | 817 |
| 068 | 568 | -1000 | -675 | 113 | 824 | 969 | 448 | -380 | -947 | -864 | -187 | 318 | 818 |
| 069 | 569 | -994 | -557 | 273 | 910 | 905 | 261 | -567 | -995 | -720 | 063 | 319 | 819 |
| 070 | 570 | -969 | -426 | 426 | 969 | 809 | 063 | -729 | -992 | -536 | 309 | 320 | 820 |
| 071 | 571 | -925 | -285 | 567 | 997 | 685 | -138 | -858 | -939 | -321 | 536 | 321 | 821 |
| 072 | 572 | -864 | -138 | 694 | 995 | 536 | -333 | -947 | -838 | -088 | 729 | 322 | 822 |
| 073 | 573 | -786 | 013 | 802 | 962 | 368 | -514 | -994 | -694 | 150 | 876 | 323 | 823 |
| 074 | 574 | -694 | 163 | 888 | 899 | 187 | -675 | -995 | -514 | 380 | 969 | 324 | 824 |
| 075 | 575 | -588 | 309 | 951 | 809 | 000 | -809 | -951 | -309 | 588 | 1000 | 325 | 825 |
| 076 | 576 | -471 | 448 | 989 | 694 | -187 | -910 | -864 | -088 | 762 | 969 | 326 | 826 |
| 077 | 577 | -345 | 578 | 1000 | 557 | -368 | -975 | -738 | 138 | 894 | 876 | 327 | 827 |
| 078 | 578 | -212 | 694 | 985 | 403 | -536 | -1000 | -578 | 356 | 975 | 729 | 328 | 828 |
| 079 | 579 | -075 | 794 | 943 | 237 | -685 | -985 | -391 | 557 | 1000 | 536 | 329 | 829 |
| 080 | 580 | 063 | 876 | 876 | 063 | -809 | -930 | -187 | 729 | 969 | 309 | 330 | 830 |
| 081 | 581 | 200 | 939 | 786 | -113 | -905 | -838 | 025 | 864 | 882 | 063 | 331 | 831 |
| 082 | 582 | 333 | 980 | 675 | -285 | -969 | -712 | 237 | 955 | 746 | -187 | 332 | 832 |
| 083 | 583 | 460 | 999 | 546 | -448 | -998 | -557 | 437 | 997 | 567 | -426 | 333 | 833 |
| 084 | 584 | 578 | 995 | 403 | -598 | -992 | -380 | 618 | 989 | 356 | -637 | 334 | 834 |
| 085 | 585 | 685 | 969 | 249 | -729 | -951 | -187 | 771 | 930 | 125 | -809 | 335 | 835 |
| 086 | 586 | 778 | 920 | 088 | -838 | -876 | 013 | 888 | 824 | -113 | -930 | 336 | 836 |
| 087 | 587 | 858 | 851 | -075 | -920 | -771 | 212 | 965 | 675 | -345 | -992 | 337 | 837 |
| 088 | 588 | 920 | 762 | -237 | -975 | -637 | 403 | 999 | 493 | -557 | -992 | 338 | 838 |
| 089 | 589 | 965 | 657 | -391 | -999 | -482 | 578 | 987 | 285 | -738 | -930 | 339 | 839 |

TABLE 8.5D (continued)

 $\cos 2\pi hx$ (h even) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=2$ | 4 | 6 | 8 | 10 | 12 | 14 | 16 | 18 | 20 | Change sign for $h=4n+2$
Sign as given for $h=4n$
x | |
|-----------------------|-----|-------|-------|------|------|------|-------|-------|-------|------|-------|---|-----|
| 090 | 590 | 426 | -637 | -969 | -187 | 809 | 876 | -063 | -930 | -729 | 309 | 340 | 840 |
| 091 | 591 | 414 | -657 | -959 | -138 | 844 | 838 | -150 | -962 | -647 | 426 | 341 | 841 |
| 092 | 592 | 403 | -675 | -947 | -088 | 876 | 794 | -237 | -985 | -557 | 536 | 342 | 842 |
| 093 | 593 | 391 | -694 | -934 | -038 | 905 | 746 | -321 | -997 | -460 | 637 | 343 | 843 |
| 094 | 594 | 380 | -712 | -920 | 013 | 930 | 694 | -403 | -1000 | -356 | 729 | 344 | 844 |
| 095 | 595 | 368 | -729 | -905 | 063 | 951 | 637 | -482 | -992 | -249 | 809 | 345 | 845 |
| 096 | 596 | 356 | -746 | -888 | 113 | 969 | 578 | -557 | -975 | -138 | 876 | 346 | 846 |
| 097 | 597 | 345 | -762 | -870 | 163 | 982 | 514 | -628 | -947 | -025 | 930 | 347 | 847 |
| 098 | 598 | 333 | -778 | -851 | 212 | 992 | 448 | -694 | -910 | 088 | 969 | 348 | 848 |
| 099 | 599 | 321 | -794 | -831 | 261 | 998 | 380 | -754 | -864 | 200 | 992 | 349 | 849 |
| 100 | 600 | 309 | -809 | -809 | 309 | 1000 | 309 | -809 | -809 | 309 | 1000 | 350 | 850 |
| 101 | 601 | 297 | -824 | -786 | 356 | 998 | 237 | -858 | -746 | 414 | 992 | 351 | 851 |
| 102 | 602 | 285 | -838 | -762 | 403 | 992 | 163 | -899 | -675 | 514 | 969 | 352 | 852 |
| 103 | 603 | 273 | -851 | -738 | 448 | 982 | 088 | -934 | -598 | 608 | 930 | 353 | 853 |
| 104 | 604 | 261 | -864 | -712 | 493 | 969 | 013 | -962 | -514 | 694 | 876 | 354 | 854 |
| 105 | 605 | 249 | -876 | -685 | 536 | 951 | -063 | -982 | -426 | 771 | 809 | 355 | 855 |
| 106 | 606 | 237 | -888 | -657 | 578 | 930 | -138 | -995 | -333 | 838 | 729 | 356 | 856 |
| 107 | 607 | 224 | -899 | -628 | 618 | 905 | -212 | -1000 | -237 | 894 | 637 | 357 | 857 |
| 108 | 608 | 212 | -910 | -598 | 657 | 876 | -285 | -997 | -138 | 939 | 536 | 358 | 858 |
| 109 | 609 | 200 | -920 | -567 | 694 | 844 | -356 | -987 | -038 | 972 | 426 | 359 | 859 |
| 110 | 610 | 187 | -930 | -536 | 729 | 809 | -426 | -969 | 063 | 992 | 309 | 360 | 860 |
| 111 | 611 | 175 | -939 | -504 | 762 | 771 | -493 | -943 | 163 | 1000 | 187 | 361 | 861 |
| 112 | 612 | 163 | -947 | -471 | 794 | 729 | -557 | -910 | 261 | 995 | 063 | 362 | 862 |
| 113 | 613 | 150 | -955 | -437 | 824 | 685 | -618 | -870 | 356 | 977 | -063 | 363 | 863 |
| 114 | 614 | 138 | -962 | -403 | 851 | 637 | -675 | -824 | 448 | 947 | -187 | 364 | 864 |
| 115 | 615 | 125 | -969 | -368 | 876 | 588 | -729 | -771 | 536 | 905 | -309 | 365 | 865 |
| 116 | 616 | 113 | -975 | -333 | 899 | 536 | -778 | -712 | 618 | 851 | -426 | 366 | 866 |
| 117 | 617 | 100 | -980 | -297 | 920 | 482 | -824 | -647 | 694 | 786 | -536 | 367 | 867 |
| 118 | 618 | 088 | -985 | -261 | 939 | 426 | -864 | -578 | 762 | 712 | -637 | 368 | 868 |
| 119 | 619 | 075 | -989 | -224 | 955 | 368 | -899 | -504 | 824 | 628 | -729 | 369 | 869 |
| 120 | 620 | 063 | -992 | -187 | 969 | 309 | -930 | -426 | 876 | 536 | -809 | 370 | 870 |
| 121 | 621 | 050 | -995 | -150 | 980 | 249 | -955 | -345 | 920 | 437 | -876 | 371 | 871 |
| 122 | 622 | 038 | -997 | -113 | 989 | 187 | -975 | -261 | 955 | 333 | -930 | 372 | 872 |
| 123 | 623 | 025 | -999 | -075 | 995 | 125 | -989 | -175 | 980 | 224 | -969 | 373 | 873 |
| 124 | 624 | 013 | -1000 | -038 | 999 | 063 | -997 | -088 | 995 | 113 | -992 | 374 | 874 |
| 125 | 625 | 000 | -1000 | 000 | 1000 | 000 | -1000 | 000 | 1000 | 000 | -1000 | 375 | 875 |
| 126 | 626 | -013 | -1000 | 038 | 999 | -063 | -997 | 088 | 995 | -113 | -992 | 376 | 876 |
| 127 | 627 | -025 | -999 | 075 | 995 | -125 | -989 | 175 | 980 | -224 | -969 | 377 | 877 |
| 128 | 628 | -038 | -997 | 113 | 989 | -187 | -975 | 261 | 955 | -333 | -930 | 378 | 878 |
| 129 | 629 | -050 | -995 | 150 | 980 | -249 | -955 | 345 | 920 | -437 | -876 | 379 | 879 |
| 130 | 630 | -063 | -992 | 187 | 969 | -309 | -930 | 426 | 876 | -536 | -809 | 380 | 880 |
| 131 | 631 | -075 | -989 | 224 | 955 | -368 | -899 | 504 | 824 | -628 | -729 | 381 | 881 |
| 132 | 632 | -088 | -985 | 261 | 939 | -426 | -864 | 578 | 762 | -712 | -637 | 382 | 882 |
| 133 | 633 | -100 | -980 | 297 | 920 | -482 | -824 | 647 | 694 | -786 | -536 | 383 | 883 |
| 134 | 634 | -113 | -975 | 333 | 899 | -536 | -778 | 712 | 618 | -851 | -426 | 384 | 884 |

TABLE 8.5D (continued)

 $\cos 2\pi hx$ (h even) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=22$ | 24 | 26 | 28 | 30 | 32 | 34 | 36 | 38 | 40 | Change sign for $h=4n+2$
Sign as given for $h=4n$
x | |
|-----------------------|-----|--------|-------|-------|-------|------|------|-------|------|-------|------|---|-----|
| 090 | 590 | 992 | 536 | -536 | -992 | -309 | 729 | 930 | 063 | -876 | -809 | 340 | 840 |
| 091 | 591 | 1000 | 403 | -666 | -955 | -125 | 851 | 831 | -163 | -965 | -637 | 341 | 841 |
| 092 | 592 | 989 | 261 | -778 | -888 | 063 | 939 | 694 | -380 | -1000 | -426 | 342 | 842 |
| 093 | 593 | 959 | 113 | -870 | -794 | 249 | 989 | 525 | -578 | -977 | -187 | 343 | 843 |
| 094 | 594 | 910 | -038 | -939 | -675 | 426 | 999 | 333 | -746 | -899 | 063 | 344 | 844 |
| | | | | | | | | | | | | | |
| 095 | 595 | 844 | -187 | -982 | -536 | 588 | 969 | 125 | -876 | -771 | 309 | 345 | 845 |
| 096 | 596 | 762 | -333 | -1000 | -380 | 729 | 899 | -088 | -962 | -598 | 536 | 346 | 846 |
| 097 | 597 | 666 | -471 | -990 | -212 | 844 | 794 | -297 | -999 | -391 | 729 | 347 | 847 |
| 098 | 598 | 557 | -598 | -955 | -038 | 930 | 657 | -493 | -985 | -163 | 876 | 348 | 848 |
| 099 | 599 | 437 | -712 | -894 | 138 | 982 | 493 | -666 | -920 | 075 | 969 | 349 | 849 |
| | | | | | | | | | | | | | |
| 100 | 600 | 309 | -809 | -809 | 309 | 1000 | 309 | -809 | -809 | 309 | 1000 | 350 | 850 |
| 101 | 601 | 175 | -888 | -703 | 471 | 982 | 113 | -915 | -657 | 525 | 969 | 351 | 851 |
| 102 | 602 | 038 | -947 | -578 | 618 | 930 | -088 | -980 | -471 | 712 | 876 | 352 | 852 |
| 103 | 603 | -100 | -985 | -437 | 746 | 844 | -285 | -1000 | -261 | 858 | 729 | 353 | 853 |
| 104 | 604 | -237 | -1000 | -285 | 851 | 729 | -471 | -975 | -038 | 955 | 536 | 354 | 854 |
| | | | | | | | | | | | | | |
| 105 | 605 | -368 | -992 | -125 | 930 | 588 | -637 | -905 | 187 | 998 | 309 | 355 | 855 |
| 106 | 606 | -493 | -962 | 038 | 980 | 426 | -778 | -794 | 403 | 985 | 063 | 356 | 856 |
| 107 | 607 | -608 | -910 | 200 | 1000 | 249 | -888 | -647 | 598 | 915 | -187 | 357 | 857 |
| 108 | 608 | -712 | -838 | 356 | 989 | 063 | -962 | -471 | 762 | 794 | -426 | 358 | 858 |
| 109 | 609 | -802 | -746 | 504 | 947 | -125 | -997 | -273 | 888 | 628 | -637 | 359 | 859 |
| | | | | | | | | | | | | | |
| 110 | 610 | -876 | -637 | 637 | 876 | -309 | -992 | -063 | 969 | 426 | -809 | 360 | 860 |
| 111 | 611 | -934 | -514 | 754 | 778 | -482 | -947 | 150 | 1000 | 200 | -930 | 361 | 861 |
| 112 | 612 | -975 | -380 | 851 | 657 | -637 | -864 | 356 | 980 | -038 | -992 | 362 | 862 |
| 113 | 613 | -996 | -237 | 925 | 514 | -771 | -746 | 546 | 910 | -273 | -992 | 363 | 863 |
| 114 | 614 | -999 | -088 | 975 | 356 | -876 | -598 | 712 | 794 | -493 | -930 | 364 | 864 |
| | | | | | | | | | | | | | |
| 115 | 615 | -982 | 063 | 998 | 187 | -951 | -426 | 844 | 637 | -685 | -809 | 365 | 865 |
| 116 | 616 | -947 | 212 | 995 | 013 | -992 | -237 | 939 | 448 | -838 | -637 | 366 | 866 |
| 117 | 617 | -894 | 356 | 965 | -163 | -998 | -038 | 990 | 237 | -943 | -426 | 367 | 867 |
| 118 | 618 | -824 | 493 | 910 | -333 | -969 | 163 | 997 | 013 | -995 | -187 | 368 | 868 |
| 119 | 619 | -738 | 618 | 831 | -493 | -905 | 356 | 959 | -212 | -990 | 063 | 369 | 869 |
| | | | | | | | | | | | | | |
| 120 | 620 | -637 | 729 | 729 | -637 | -809 | 536 | 876 | -426 | -930 | 309 | 370 | 870 |
| 121 | 621 | -525 | 824 | 608 | -762 | -685 | 694 | 754 | -618 | -816 | 536 | 371 | 871 |
| 122 | 622 | -403 | 899 | 471 | -864 | -536 | 824 | 598 | -778 | -657 | 729 | 372 | 872 |
| 123 | 623 | -273 | 955 | 321 | -939 | -368 | 920 | 414 | -899 | -460 | 876 | 373 | 873 |
| 124 | 624 | -138 | 989 | 163 | -985 | -187 | 980 | 212 | -975 | -237 | 969 | 374 | 874 |
| | | | | | | | | | | | | | |
| 125 | 625 | 000 | 1000 | 000 | -1000 | 000 | 1000 | 000 | 1000 | 000 | 1000 | 375 | 875 |
| 126 | 626 | 138 | 989 | -163 | -985 | 187 | 980 | -212 | -975 | 237 | 969 | 376 | 876 |
| 127 | 627 | 273 | 955 | -321 | -939 | 368 | 920 | -414 | -899 | 460 | 876 | 377 | 877 |
| 128 | 628 | 403 | 899 | -471 | -864 | 536 | 824 | -598 | -778 | 657 | 729 | 378 | 878 |
| 129 | 629 | 525 | 824 | -608 | -762 | 685 | 694 | -754 | -618 | 816 | 536 | 379 | 879 |
| | | | | | | | | | | | | | |
| 130 | 630 | 637 | 729 | -729 | -637 | 809 | 536 | -876 | -426 | 930 | 309 | 380 | 880 |
| 131 | 631 | 738 | 618 | -831 | -493 | 905 | 356 | -959 | -212 | 990 | 063 | 381 | 881 |
| 132 | 632 | 824 | 493 | -910 | -333 | 969 | 163 | -997 | 013 | 995 | -187 | 382 | 882 |
| 133 | 633 | 894 | 356 | -965 | -163 | 998 | -038 | -990 | 237 | 943 | -426 | 383 | 883 |
| 134 | 634 | 947 | 212 | -995 | 013 | 992 | -237 | -939 | 448 | 838 | -637 | 384 | 884 |

TABLE 8.5D (continued)

 $\cos 2\pi hx$ (h even) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=2$ | 4 | 6 | 8 | 10 | 12 | 14 | 16 | 18 | 20 | Change sign for $h=4n+2$
Sign as given for $h=4n$
x | |
|-----------------------|-----|-------|------|------|------|-------|------|------|-------|-------|-------|---|-----|
| 135 | 635 | -125 | -969 | 368 | 876 | -588 | -729 | 771 | 536 | -905 | -309 | 385 | 885 |
| 136 | 636 | -138 | -962 | 403 | 851 | -637 | -675 | 824 | 448 | -947 | -187 | 386 | 886 |
| 137 | 637 | -150 | -955 | 437 | 824 | -685 | -618 | 870 | 356 | -977 | -063 | 387 | 887 |
| 138 | 638 | -163 | -947 | 471 | 794 | -729 | -557 | 910 | 261 | -995 | 063 | 388 | 888 |
| 139 | 639 | -175 | -939 | 504 | 762 | -771 | -493 | 943 | 163 | -1000 | 187 | 389 | 889 |
| 140 | 640 | -187 | -930 | 536 | 729 | -809 | -426 | 969 | 063 | -992 | 309 | 390 | 890 |
| 141 | 641 | -200 | -920 | 567 | 694 | -844 | -356 | 987 | -038 | -972 | 426 | 391 | 891 |
| 142 | 642 | -212 | -910 | 598 | 657 | -876 | -285 | 997 | -138 | -939 | 536 | 392 | 892 |
| 143 | 643 | -224 | -899 | 628 | 618 | -905 | -212 | 1000 | -237 | -894 | 637 | 393 | 893 |
| 144 | 644 | -237 | -888 | 657 | 578 | -930 | -138 | 995 | -333 | -838 | 729 | 394 | 894 |
| 145 | 645 | -249 | -876 | 685 | 536 | -951 | -063 | 982 | -426 | -771 | 809 | 395 | 895 |
| 146 | 646 | -261 | -864 | 712 | 493 | -969 | 013 | 962 | -514 | -694 | 876 | 396 | 896 |
| 147 | 647 | -273 | -851 | 737 | 448 | -982 | 088 | 934 | -598 | -608 | 930 | 397 | 897 |
| 148 | 648 | -285 | -838 | 762 | 403 | -992 | 163 | 899 | -675 | -514 | 969 | 398 | 898 |
| 149 | 649 | -297 | -824 | 786 | 356 | -998 | 237 | 858 | -746 | -414 | 992 | 399 | 899 |
| 150 | 650 | -309 | -809 | 809 | 309 | -1000 | 309 | 809 | -809 | -309 | 1000 | 400 | 900 |
| 151 | 651 | -321 | -794 | 831 | 261 | -998 | 380 | 754 | -864 | -200 | 992 | 401 | 901 |
| 152 | 652 | -333 | -778 | 851 | 212 | -992 | 448 | 694 | -910 | -088 | 969 | 402 | 902 |
| 153 | 653 | -345 | -762 | 870 | 163 | -982 | 514 | 628 | -947 | 025 | 930 | 403 | 903 |
| 154 | 654 | -356 | -746 | 888 | 113 | -969 | 578 | 557 | -975 | 138 | 876 | 404 | 904 |
| 155 | 655 | -368 | -729 | 905 | 063 | -951 | 637 | 482 | -992 | 249 | 809 | 405 | 905 |
| 156 | 656 | -380 | -712 | 920 | 013 | -930 | 694 | 403 | -1000 | 356 | 729 | 406 | 906 |
| 157 | 657 | -391 | -694 | 934 | -038 | -905 | 746 | 321 | -997 | 460 | 637 | 407 | 907 |
| 158 | 658 | -403 | -675 | 947 | -088 | -876 | 794 | 237 | -985 | 557 | 536 | 408 | 908 |
| 159 | 659 | -414 | -657 | 959 | -138 | -844 | 838 | 150 | -962 | 647 | 426 | 409 | 909 |
| 160 | 660 | -426 | -637 | 969 | -187 | -809 | 876 | 063 | -930 | 729 | 309 | 410 | 910 |
| 161 | 661 | -437 | -618 | 977 | -237 | -771 | 910 | -025 | -888 | 802 | 187 | 411 | 911 |
| 162 | 662 | -448 | -598 | 985 | -285 | -729 | 939 | -113 | -838 | 864 | 063 | 412 | 912 |
| 163 | 663 | -460 | -578 | 990 | -333 | -685 | 962 | -200 | -778 | 915 | -063 | 413 | 913 |
| 164 | 664 | -471 | -557 | 995 | -380 | -637 | 980 | -285 | -712 | 955 | -187 | 414 | 914 |
| 165 | 665 | -482 | -536 | 998 | -426 | -588 | 992 | -368 | -637 | 982 | -309 | 415 | 915 |
| 166 | 666 | -493 | -514 | 1000 | -471 | -536 | 999 | -448 | -557 | 997 | -426 | 416 | 916 |
| 167 | 667 | -504 | -493 | 1000 | -514 | -482 | 1000 | -525 | -471 | 999 | -536 | 417 | 917 |
| 168 | 668 | -514 | -471 | 999 | -557 | -426 | 995 | -598 | -380 | 989 | -637 | 418 | 918 |
| 169 | 669 | -525 | -448 | 996 | -598 | -368 | 985 | -666 | -285 | 965 | -729 | 419 | 919 |
| 170 | 670 | -536 | -426 | 992 | -637 | -309 | 969 | -729 | -187 | 930 | -809 | 420 | 920 |
| 171 | 671 | -546 | -403 | 987 | -675 | -249 | 947 | -786 | -088 | 882 | -876 | 421 | 921 |
| 172 | 672 | -557 | -380 | 980 | -712 | -187 | 920 | -838 | 013 | 824 | -930 | 422 | 922 |
| 173 | 673 | -567 | -356 | 972 | -746 | -125 | 888 | -882 | 113 | 754 | -969 | 423 | 923 |
| 174 | 674 | -578 | -333 | 962 | -778 | -063 | 851 | -920 | 212 | 675 | -992 | 424 | 924 |
| 175 | 675 | -588 | -309 | 951 | -809 | 000 | 809 | -951 | 309 | 588 | -1000 | 425 | 925 |
| 176 | 676 | -598 | -285 | 939 | -838 | 063 | 762 | -975 | 403 | 493 | -992 | 426 | 926 |
| 177 | 677 | -608 | -261 | 925 | -864 | 125 | 712 | -990 | 493 | 391 | -969 | 427 | 927 |
| 178 | 678 | -618 | -237 | 910 | -888 | 187 | 657 | -999 | 578 | 285 | -930 | 428 | 928 |
| 179 | 679 | -628 | -212 | 894 | -910 | 249 | 598 | -999 | 657 | 175 | -876 | 429 | 929 |

TABLE 8.5D (continued)

 $\cos 2\pi hx$ (h even) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=22$ | 24 | 26 | 28 | 30 | 32 | 34 | 36 | 38 | 40 | Change sign for $h=4n+2$
Sign as given for $h=4n$
x | |
|-----------------------|-----|--------|-------|-------|------|-------|-------|------|------|-------|------|---|-----|
| 135 | 635 | 982 | 063 | -998 | 187 | 951 | -426 | -844 | 637 | 685 | -809 | 385 | 885 |
| 136 | 636 | 999 | -088 | -975 | 356 | 876 | -598 | -712 | 794 | 493 | -930 | 386 | 886 |
| 137 | 637 | 996 | -237 | -925 | 514 | 771 | -746 | -546 | 910 | 273 | -992 | 387 | 887 |
| 138 | 638 | 975 | -380 | -851 | 657 | 637 | -864 | -356 | 980 | 038 | -992 | 388 | 888 |
| 139 | 639 | 934 | -514 | -754 | 778 | 482 | -947 | -150 | 1000 | -200 | -930 | 389 | 889 |
| 140 | 640 | 876 | -637 | -637 | 876 | 309 | -992 | 063 | 969 | -426 | -809 | 390 | 890 |
| 141 | 641 | 802 | -746 | -504 | 947 | 125 | -997 | 273 | 888 | -628 | -637 | 391 | 891 |
| 142 | 642 | 712 | -838 | -356 | 989 | -063 | -962 | 471 | 762 | -794 | -426 | 392 | 892 |
| 143 | 643 | 608 | -910 | -200 | 1000 | -249 | -888 | 647 | 598 | -915 | -187 | 393 | 893 |
| 144 | 644 | 493 | -962 | -038 | 980 | -426 | -778 | 794 | 403 | -985 | 063 | 394 | 894 |
| 145 | 645 | 368 | -992 | 125 | 930 | -588 | -637 | 905 | 187 | -998 | 309 | 395 | 895 |
| 146 | 646 | 237 | -1000 | 285 | 851 | -729 | -471 | 975 | -038 | -955 | 536 | 396 | 896 |
| 147 | 647 | 100 | -985 | 437 | 746 | -844 | -285 | 1000 | -261 | -858 | 729 | 397 | 897 |
| 148 | 648 | -038 | -947 | 578 | 618 | -930 | -088 | 980 | -471 | -712 | 876 | 398 | 898 |
| 149 | 649 | -175 | -888 | 703 | 471 | -982 | 113 | 915 | -657 | -525 | 969 | 399 | 899 |
| 150 | 650 | -309 | -809 | 809 | 309 | -1000 | 309 | 809 | -809 | -309 | 1000 | 400 | 900 |
| 151 | 651 | -437 | -712 | 894 | 138 | -982 | 493 | 666 | -920 | -075 | 969 | 401 | 901 |
| 152 | 652 | -557 | -598 | 955 | -038 | -930 | 657 | 493 | -985 | 163 | 876 | 402 | 902 |
| 153 | 653 | -666 | -471 | 990 | -212 | -844 | 794 | 297 | -999 | 391 | 729 | 403 | 903 |
| 154 | 654 | -762 | -333 | 1000 | -380 | -729 | 899 | 088 | -962 | 598 | 536 | 404 | 904 |
| 155 | 655 | -844 | -187 | 982 | -536 | -588 | 969 | -125 | -876 | 771 | 309 | 405 | 905 |
| 156 | 656 | -910 | -038 | 939 | -675 | -426 | 999 | -333 | -746 | 899 | 063 | 406 | 906 |
| 157 | 657 | -959 | 113 | 870 | -794 | -249 | 989 | -525 | -578 | 977 | -187 | 407 | 907 |
| 158 | 658 | -989 | 261 | 778 | -888 | -063 | 939 | -694 | -380 | 1000 | -426 | 408 | 908 |
| 159 | 659 | -1000 | 403 | 666 | -955 | 125 | 851 | -831 | -163 | 965 | -637 | 409 | 909 |
| 160 | 660 | -992 | 536 | 536 | -992 | 309 | 729 | -930 | 063 | 876 | -809 | 410 | 910 |
| 161 | 661 | -965 | 657 | 391 | -999 | 482 | 578 | -987 | 285 | 738 | -930 | 411 | 911 |
| 162 | 662 | -920 | 762 | 237 | -975 | 637 | 403 | -999 | 493 | 557 | -992 | 412 | 912 |
| 163 | 663 | -858 | 851 | 075 | -920 | 771 | 212 | -965 | 675 | 345 | -992 | 413 | 913 |
| 164 | 664 | -778 | 920 | -088 | -838 | 876 | 013 | -888 | 824 | 113 | -930 | 414 | 914 |
| 165 | 665 | -685 | 969 | -249 | -729 | 951 | -187 | -771 | 930 | -125 | -809 | 415 | 915 |
| 166 | 666 | -578 | 995 | -403 | -598 | 992 | -380 | -618 | 989 | -356 | -637 | 416 | 916 |
| 167 | 667 | -460 | 999 | -546 | -448 | 998 | -557 | -437 | 997 | -567 | -426 | 417 | 917 |
| 168 | 668 | -333 | 980 | -675 | -285 | 969 | -712 | -237 | 955 | -746 | -187 | 418 | 918 |
| 169 | 669 | -200 | 939 | -786 | -113 | 905 | -838 | -025 | 864 | -882 | 063 | 419 | 919 |
| 170 | 670 | -063 | 876 | -876 | 063 | 809 | -930 | 187 | 729 | -969 | 309 | 420 | 920 |
| 171 | 671 | 075 | 794 | -943 | 237 | 685 | -985 | 391 | 557 | -1000 | 536 | 421 | 921 |
| 172 | 672 | 212 | 694 | -985 | 403 | 536 | -1000 | 578 | 356 | -975 | 729 | 422 | 922 |
| 173 | 673 | 345 | 578 | -1000 | 557 | 368 | -975 | 737 | 138 | -894 | 876 | 423 | 923 |
| 174 | 674 | 471 | 448 | -989 | 694 | 187 | -910 | 864 | -088 | -762 | 969 | 424 | 924 |
| 175 | 675 | 588 | 309 | -951 | 809 | 000 | -809 | 951 | -309 | -588 | 1000 | 425 | 925 |
| 176 | 676 | 694 | 163 | -888 | 899 | -187 | -675 | 995 | -514 | -380 | 969 | 426 | 926 |
| 177 | 677 | 786 | 013 | -802 | 962 | -368 | -514 | 994 | -694 | -150 | 876 | 427 | 927 |
| 178 | 678 | 864 | -138 | -694 | 995 | -536 | -333 | 947 | -838 | 088 | 729 | 428 | 928 |
| 179 | 679 | 925 | -285 | -567 | 997 | -685 | -138 | 858 | -939 | 321 | 536 | 429 | 929 |

TABLE 8.5D (continued)

 $\cos 2\pi hx$ (h even) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=2$ | 4 | 6 | 8 | 10 | 12 | 14 | 16 | 18 | 20 | Change sign for $h=4n+2$
Sign as given for $h=4n$
x | |
|-----------------------|-----|-------|------|------|-------|------|-------|------|-------|------|------|---|-----|
| 180 | 680 | -637 | -187 | 876 | -930 | 309 | 536 | -992 | 729 | 063 | -809 | 430 | 930 |
| 181 | 681 | -647 | -163 | 858 | -947 | 368 | 471 | -977 | 794 | -050 | -729 | 431 | 931 |
| 182 | 682 | -657 | -138 | 838 | -962 | 426 | 403 | -955 | 851 | -163 | -637 | 432 | 932 |
| 183 | 683 | -666 | -113 | 816 | -975 | 482 | 333 | -925 | 899 | -273 | -536 | 433 | 933 |
| 184 | 684 | -675 | -088 | 794 | -985 | 536 | 261 | -888 | 939 | -380 | -426 | 434 | 934 |
| 185 | 685 | -685 | -063 | 771 | -992 | 588 | 187 | -844 | 969 | -482 | -309 | 435 | 935 |
| 186 | 686 | -694 | -038 | 746 | -997 | 637 | 113 | -794 | 989 | -578 | -187 | 436 | 936 |
| 187 | 687 | -703 | -013 | 720 | -1000 | 685 | 038 | -738 | 999 | -666 | -063 | 437 | 937 |
| 188 | 688 | -712 | 013 | 694 | -1000 | 729 | -038 | -675 | 999 | -746 | 063 | 438 | 938 |
| 189 | 689 | -720 | 038 | 666 | -997 | 771 | -113 | -608 | 989 | -816 | 187 | 439 | 939 |
| 190 | 690 | -729 | 063 | 637 | -992 | 809 | -187 | -536 | 969 | -876 | 309 | 440 | 940 |
| 191 | 691 | -738 | 088 | 608 | -985 | 844 | -261 | -460 | 939 | -925 | 426 | 441 | 941 |
| 192 | 692 | -746 | 113 | 578 | -975 | 876 | -333 | -380 | 899 | -962 | 536 | 442 | 942 |
| 193 | 693 | -754 | 138 | 546 | -962 | 905 | -403 | -297 | 851 | -987 | 637 | 443 | 943 |
| 194 | 694 | -762 | 163 | 514 | -947 | 930 | -471 | -212 | 794 | -999 | 729 | 444 | 944 |
| 195 | 695 | -771 | 187 | 482 | -930 | 951 | -536 | -125 | 729 | -998 | 809 | 445 | 945 |
| 196 | 696 | -778 | 212 | 448 | -910 | 969 | -598 | -038 | 657 | -985 | 876 | 446 | 946 |
| 197 | 697 | -786 | 237 | 414 | -888 | 982 | -657 | 050 | 578 | -959 | 930 | 447 | 947 |
| 198 | 698 | -794 | 261 | 380 | -864 | 992 | -712 | 138 | 493 | -920 | 969 | 448 | 948 |
| 199 | 699 | -802 | 285 | 345 | -838 | 998 | -762 | 224 | 403 | -870 | 992 | 449 | 949 |
| 200 | 700 | -809 | 309 | 309 | -809 | 1000 | -809 | 309 | 309 | -809 | 1000 | 450 | 950 |
| 201 | 701 | -816 | 333 | 273 | -778 | 998 | -851 | 391 | 212 | -738 | 992 | 451 | 951 |
| 202 | 702 | -824 | 356 | 237 | -746 | 992 | -888 | 471 | 113 | -657 | 969 | 452 | 952 |
| 203 | 703 | -831 | 380 | 200 | -712 | 982 | -920 | 546 | 013 | -567 | 930 | 453 | 953 |
| 204 | 704 | -838 | 403 | 163 | -675 | 969 | -947 | 618 | -088 | -471 | 876 | 454 | 954 |
| 205 | 705 | -844 | 426 | 125 | -637 | 951 | -969 | 685 | -187 | -368 | 809 | 455 | 955 |
| 206 | 706 | -851 | 448 | 088 | -598 | 930 | -985 | 746 | -285 | -261 | 729 | 456 | 956 |
| 207 | 707 | -858 | 471 | 050 | -557 | 905 | -995 | 802 | -380 | -150 | 637 | 457 | 957 |
| 208 | 708 | -864 | 493 | 013 | -514 | 876 | -1000 | 851 | -471 | -038 | 536 | 458 | 958 |
| 209 | 709 | -870 | 514 | -025 | -471 | 844 | -999 | 894 | -557 | 075 | 426 | 459 | 959 |
| 210 | 710 | -876 | 536 | -063 | -426 | 809 | -992 | 930 | -637 | 187 | 309 | 460 | 960 |
| 211 | 711 | -882 | 557 | -100 | -380 | 771 | -980 | 959 | -712 | 297 | 187 | 461 | 961 |
| 212 | 712 | -888 | 578 | -138 | -333 | 729 | -962 | 980 | -778 | 403 | 063 | 462 | 962 |
| 213 | 713 | -894 | 598 | -175 | -285 | 685 | -939 | 994 | -838 | 504 | -063 | 463 | 963 |
| 214 | 714 | -899 | 618 | -212 | -237 | 637 | -910 | 1000 | -888 | 598 | -187 | 464 | 964 |
| 215 | 715 | -905 | 637 | -249 | -187 | 588 | -876 | 998 | -930 | 685 | -309 | 465 | 965 |
| 216 | 716 | -910 | 657 | -285 | -138 | 536 | -838 | 989 | -962 | 762 | -426 | 466 | 966 |
| 217 | 717 | -915 | 675 | -321 | -088 | 482 | -794 | 972 | -985 | 831 | -536 | 467 | 967 |
| 218 | 718 | -920 | 694 | -356 | -038 | 426 | -746 | 947 | -997 | 888 | -637 | 468 | 968 |
| 219 | 719 | -925 | 712 | -391 | 013 | 368 | -694 | 915 | -1000 | 934 | -729 | 469 | 969 |
| 220 | 720 | -930 | 729 | -426 | 063 | 309 | -637 | 876 | -992 | 969 | -809 | 470 | 970 |
| 221 | 721 | -934 | 746 | -460 | 113 | 249 | -578 | 831 | -975 | 990 | -876 | 471 | 971 |
| 222 | 722 | -939 | 762 | -493 | 163 | 187 | -514 | 778 | -947 | 1000 | -930 | 472 | 972 |
| 223 | 723 | -943 | 778 | -525 | 212 | 125 | -448 | 720 | -910 | 996 | -969 | 473 | 973 |
| 224 | 724 | -947 | 794 | -557 | 261 | 063 | -380 | 657 | -864 | 980 | -992 | 474 | 974 |

TABLE 8.5D (continued)

 $\cos 2\pi hx$ (h even) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=22$ | 24 | 26 | 28 | 30 | 32 | 34 | 36 | 38 | 40 | Change sign for $h=4n+2$
Sign as given for $h=4n$
x | |
|-----------------------|-----|--------|------|------|------|------|-------|------|------|------|------|---|-----|
| 180 | 680 | 969 | -426 | -426 | 969 | -809 | 063 | 729 | -992 | 536 | 309 | 430 | 930 |
| 181 | 681 | 994 | -557 | -273 | 910 | -905 | 261 | 567 | -995 | 720 | 063 | 431 | 931 |
| 182 | 682 | 1000 | -675 | -113 | 824 | -969 | 448 | 380 | -947 | 864 | -187 | 432 | 932 |
| 183 | 683 | 987 | -778 | 050 | 712 | -998 | 618 | 175 | -851 | 959 | -426 | 433 | 933 |
| 184 | 684 | 955 | -864 | 212 | 578 | -992 | 762 | -038 | -712 | 999 | -637 | 434 | 934 |
| 185 | 685 | 905 | -930 | 368 | 426 | -951 | 876 | -249 | -536 | 982 | -809 | 435 | 935 |
| 186 | 686 | 838 | -975 | 514 | 261 | -876 | 955 | -448 | -333 | 910 | -930 | 436 | 936 |
| 187 | 687 | 754 | -997 | 647 | 088 | -771 | 995 | -628 | -113 | 786 | -992 | 437 | 937 |
| 188 | 688 | 657 | -997 | 762 | -088 | -637 | 995 | -778 | 113 | 618 | -992 | 438 | 938 |
| 189 | 689 | 546 | -975 | 858 | -261 | -482 | 955 | -894 | 333 | 414 | -930 | 439 | 939 |
| 190 | 690 | 426 | -930 | 930 | -426 | -309 | 876 | -969 | 536 | 187 | -809 | 440 | 940 |
| 191 | 691 | 297 | -864 | 977 | -578 | -125 | 762 | -999 | 712 | -050 | -637 | 441 | 941 |
| 192 | 692 | 163 | -778 | 999 | -712 | 063 | 618 | -985 | 851 | -285 | -426 | 442 | 942 |
| 193 | 693 | 025 | -675 | 994 | -824 | 249 | 448 | -925 | 947 | -504 | -187 | 443 | 943 |
| 194 | 694 | -113 | -557 | 962 | -910 | 426 | 261 | -824 | 995 | -694 | 063 | 444 | 944 |
| 195 | 695 | -249 | -426 | 905 | -969 | 588 | 063 | -685 | 992 | -844 | 309 | 445 | 945 |
| 196 | 696 | -380 | -285 | 824 | -997 | 729 | -138 | -514 | 939 | -947 | 536 | 446 | 946 |
| 197 | 697 | -504 | -138 | 720 | -995 | 844 | -333 | -321 | 838 | -996 | 729 | 447 | 947 |
| 198 | 698 | -618 | 013 | 598 | -962 | 930 | -514 | -113 | 694 | -989 | 876 | 448 | 948 |
| 199 | 699 | -720 | 163 | 460 | -899 | 982 | -675 | 100 | 514 | -925 | 969 | 449 | 949 |
| 200 | 700 | -809 | 309 | 309 | -809 | 1000 | -809 | 309 | 309 | -809 | 1000 | 450 | 950 |
| 201 | 701 | -882 | 448 | 150 | -694 | 982 | -910 | 504 | 088 | -647 | 969 | 451 | 951 |
| 202 | 702 | -939 | 578 | -013 | -557 | 930 | -975 | 675 | -138 | -448 | 876 | 452 | 952 |
| 203 | 703 | -977 | 694 | -175 | -403 | 844 | -1000 | 816 | -356 | -224 | 729 | 453 | 953 |
| 204 | 704 | -997 | 794 | -333 | -237 | 729 | -985 | 920 | -557 | 013 | 536 | 454 | 954 |
| 205 | 705 | -998 | 876 | -482 | -063 | 588 | -930 | 982 | -729 | 249 | 309 | 455 | 955 |
| 206 | 706 | -980 | 939 | -618 | 113 | 426 | -838 | 1000 | -864 | 471 | 063 | 456 | 956 |
| 207 | 707 | -943 | 980 | -738 | 285 | 249 | -712 | 972 | -955 | 666 | -187 | 457 | 957 |
| 208 | 708 | -888 | 999 | -838 | 448 | 063 | -557 | 899 | -997 | 824 | -426 | 458 | 958 |
| 209 | 709 | -816 | 995 | -915 | 598 | -125 | -380 | 786 | -989 | 934 | -637 | 459 | 959 |
| 210 | 710 | -729 | 969 | -969 | 729 | -309 | -187 | 637 | -930 | 992 | -809 | 460 | 960 |
| 211 | 711 | -628 | 920 | -996 | 838 | -482 | 013 | 460 | -824 | 994 | -930 | 461 | 961 |
| 212 | 712 | -514 | 851 | -997 | 920 | -637 | 212 | 261 | -675 | 939 | -992 | 462 | 962 |
| 213 | 713 | -391 | 762 | -972 | 975 | -771 | 403 | 050 | -493 | 831 | -992 | 463 | 963 |
| 214 | 714 | -261 | 657 | -920 | 999 | -876 | 578 | -163 | -285 | 675 | -930 | 464 | 964 |
| 215 | 715 | -125 | 536 | -844 | 992 | -951 | 729 | -368 | -063 | 482 | -809 | 465 | 965 |
| 216 | 716 | 013 | 403 | -746 | 955 | -992 | 851 | -557 | 163 | 261 | -637 | 466 | 966 |
| 217 | 717 | 150 | 261 | -628 | 888 | -998 | 939 | -720 | 380 | 025 | -426 | 467 | 967 |
| 218 | 718 | 285 | 113 | -493 | 794 | -969 | 989 | -851 | 578 | -212 | -187 | 468 | 968 |
| 219 | 719 | 414 | -038 | -345 | 675 | -905 | 999 | -943 | 746 | -437 | 063 | 469 | 969 |
| 220 | 720 | 536 | -187 | -187 | 536 | -809 | 969 | -992 | 876 | -637 | 309 | 470 | 970 |
| 221 | 721 | 647 | -333 | -025 | 380 | -685 | 899 | -996 | 962 | -802 | 536 | 471 | 971 |
| 222 | 722 | 746 | -471 | 138 | 212 | -536 | 794 | -955 | 999 | -920 | 729 | 472 | 972 |
| 223 | 723 | 831 | -598 | 297 | 038 | -368 | 657 | -870 | 985 | -987 | 876 | 473 | 973 |
| 224 | 724 | 899 | -712 | 448 | -138 | -187 | 493 | -746 | 920 | -997 | 969 | 474 | 974 |

TABLE 8.5D (continued)

 $\cos 2\pi hx$ (h even) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=2$ | 4 | 6 | 8 | 10 | 12 | 14 | 16 | 18 | 20 | Change sign for $h=4n+2$
Sign as given for $h=4n$
x | |
|-----------------------|-----|-------|------|-------|------|-------|------|-------|------|-------|-------|---|------|
| 225 | 725 | -951 | 809 | -588 | 309 | 000 | -309 | 588 | -809 | 951 | -1000 | 475 | 975 |
| 226 | 726 | -955 | 824 | -618 | 356 | -063 | -237 | 514 | -746 | 910 | -992 | 476 | 976 |
| 227 | 727 | -959 | 838 | -647 | 403 | -125 | -163 | 437 | -675 | 858 | -969 | 477 | 977 |
| 228 | 728 | -962 | 851 | -675 | 448 | -187 | -088 | 356 | -598 | 794 | -930 | 478 | 978 |
| 229 | 729 | -965 | 864 | -703 | 493 | -249 | -013 | 273 | -514 | 720 | -876 | 479 | 979 |
| | | | | | | | | | | | | | |
| 230 | 730 | -969 | 876 | -729 | 536 | -309 | 063 | 187 | -426 | 637 | -809 | 480 | 980 |
| 231 | 731 | -972 | 888 | -754 | 578 | -368 | 138 | 100 | -333 | 546 | -729 | 481 | 981 |
| 232 | 732 | -975 | 899 | -778 | 618 | -426 | 212 | 013 | -237 | 448 | -637 | 482 | 982 |
| 233 | 733 | -977 | 910 | -802 | 657 | -482 | 285 | -075 | -138 | 345 | -536 | 483 | 983 |
| 234 | 734 | -980 | 920 | -824 | 694 | -536 | 356 | -163 | -038 | 237 | -426 | 484 | 984 |
| | | | | | | | | | | | | | |
| 235 | 735 | -982 | 930 | -844 | 729 | -588 | 426 | -249 | 063 | 125 | -309 | 485 | 985 |
| 236 | 736 | -985 | 939 | -864 | 762 | -637 | 493 | -333 | 163 | 013 | -187 | 486 | 986 |
| 237 | 737 | -987 | 947 | -882 | 794 | -685 | 557 | -414 | 261 | -100 | -063 | 487 | 987 |
| 238 | 738 | -989 | 955 | -899 | 824 | -729 | 618 | -493 | 356 | -212 | 063 | 488 | 988 |
| 239 | 739 | -990 | 962 | -915 | 851 | -771 | 675 | -567 | 448 | -321 | 187 | 489 | 989 |
| | | | | | | | | | | | | | |
| 240 | 740 | -992 | 969 | -930 | 876 | -809 | 729 | -637 | 536 | -426 | 309 | 490 | 990 |
| 241 | 741 | -994 | 975 | -943 | 899 | -844 | 778 | -703 | 618 | -525 | 426 | 491 | 991 |
| 242 | 742 | -995 | 980 | -955 | 920 | -876 | 824 | -762 | 694 | -618 | 536 | 492 | 992 |
| 243 | 743 | -996 | 985 | -965 | 939 | -905 | 864 | -816 | 762 | -703 | 637 | 493 | 993 |
| 244 | 744 | -997 | 989 | -975 | 955 | -930 | 899 | -864 | 824 | -778 | 729 | 494 | 994 |
| | | | | | | | | | | | | | |
| 245 | 745 | -998 | 992 | -982 | 969 | -951 | 930 | -905 | 876 | -844 | 809 | 495 | 995 |
| 246 | 746 | -999 | 995 | -989 | 980 | -969 | 955 | -939 | 920 | -899 | 876 | 496 | 996 |
| 247 | 747 | -999 | 997 | -994 | 989 | -982 | 975 | -965 | 955 | -943 | 930 | 497 | 997 |
| 248 | 748 | -1000 | 999 | -997 | 995 | -992 | 989 | -985 | 980 | -975 | 969 | 498 | 998 |
| 249 | 749 | -1000 | 1000 | -999 | 999 | -998 | 997 | -996 | 995 | -994 | 992 | 499 | 999 |
| | | | | | | | | | | | | | |
| 250 | 750 | -1000 | 1000 | -1000 | 1000 | -1000 | 1000 | -1000 | 1000 | -1000 | 1000 | 500 | 1000 |

TABLE 8.5D (continued)

$\cos 2\pi hx$ (h even) (x fractional. Decimal points omitted throughout)

| Sign as given.
x | | $h=22$ | 24 | 26 | 28 | 30 | 32 | 34 | 36 | 38 | 40 | Change sign for $h=4n+2$
Sign as given for $h=4n$
x | |
|-----------------------|-----|--------|-------|-------|-------|-------|------|-------|-------|-------|------|---|------|
| 225 | 725 | 951 | −809 | 588 | −309 | 000 | 309 | −588 | 809 | −951 | 1000 | 475 | 975 |
| 226 | 726 | 985 | −888 | 712 | −471 | 187 | 113 | −403 | 657 | −851 | 969 | 476 | 976 |
| 227 | 727 | 999 | −947 | 816 | −618 | 368 | −088 | −200 | 471 | −703 | 876 | 477 | 977 |
| 228 | 728 | 995 | −985 | 899 | −746 | 536 | −285 | 013 | 261 | −514 | 729 | 478 | 978 |
| 229 | 729 | 972 | −1000 | 959 | −851 | 685 | −471 | 224 | 038 | −297 | 536 | 479 | 979 |
| 230 | 730 | 930 | −992 | 992 | −930 | 809 | −637 | 426 | −187 | −063 | 309 | 480 | 980 |
| 231 | 731 | 870 | −962 | 999 | −980 | 905 | −778 | 608 | −403 | 175 | 063 | 481 | 981 |
| 232 | 732 | 794 | −910 | 980 | −1000 | 969 | −888 | 762 | −598 | 403 | −187 | 482 | 982 |
| 233 | 733 | 703 | −838 | 934 | −989 | 998 | −962 | 882 | −762 | 608 | −426 | 483 | 983 |
| 234 | 734 | 598 | −746 | 864 | −947 | 992 | −997 | 962 | −888 | 778 | −637 | 484 | 984 |
| 235 | 735 | 482 | −637 | 771 | −876 | 951 | −992 | 998 | −969 | 905 | −809 | 485 | 985 |
| 236 | 736 | 356 | −514 | 657 | −778 | 876 | −947 | 989 | −1000 | 980 | −930 | 486 | 986 |
| 237 | 737 | 224 | −380 | 525 | −657 | 771 | −864 | 934 | −980 | 999 | −992 | 487 | 987 |
| 238 | 738 | 088 | −237 | 380 | −514 | 637 | −746 | 838 | −910 | 962 | −992 | 488 | 988 |
| 239 | 739 | −050 | −088 | 224 | −356 | 482 | −598 | 703 | −794 | 870 | −930 | 489 | 989 |
| 240 | 740 | −187 | 063 | 063 | −187 | 309 | −426 | 536 | −637 | 729 | −809 | 490 | 990 |
| 241 | 741 | −321 | 212 | −100 | −013 | 125 | −237 | 345 | −448 | 546 | −637 | 491 | 991 |
| 242 | 742 | −448 | 356 | −261 | 163 | −063 | −038 | 138 | −237 | 333 | −426 | 492 | 992 |
| 243 | 743 | −567 | 493 | −414 | 333 | −249 | 163 | −075 | −013 | 100 | −187 | 493 | 993 |
| 244 | 744 | −675 | 618 | −557 | 493 | −426 | 356 | −285 | 212 | −138 | 063 | 494 | 994 |
| 245 | 745 | −771 | 729 | −685 | 637 | −588 | 536 | −482 | 426 | −368 | 309 | 495 | 995 |
| 246 | 746 | −851 | 824 | −794 | 762 | −729 | 694 | −657 | 618 | −578 | 536 | 496 | 996 |
| 247 | 747 | −915 | 899 | −882 | 864 | −844 | 824 | −802 | 778 | −754 | 729 | 497 | 997 |
| 248 | 748 | −962 | 955 | −947 | 939 | −930 | 920 | −910 | 899 | −888 | 876 | 498 | 998 |
| 249 | 749 | −990 | 989 | −987 | 985 | −982 | 980 | −977 | 975 | −972 | 969 | 499 | 999 |
| 250 | 750 | −1000 | 1000 | −1000 | 1000 | −1000 | 1000 | −1000 | 1000 | −1000 | 1000 | 500 | 1000 |

8.6. Conversions of Degrees to Radians, etc.

TABLE 8.6

Conversion of Degrees, Minutes and Seconds to Radians; and of Minutes and Seconds to Decimals of a Degree; and vice versa

| No. of
degrees,
minutes
or seconds | Degrees in
radians | Minutes in
decimals of
degree | Minutes in
radians | Seconds in
decimals of
degree | Seconds in
radians
$\times 10^6$ | No. |
|---|-----------------------|-------------------------------------|-----------------------|-------------------------------------|--|-----|
| 1 | 0.01745 | 0.01667 | 0.00029 | 0.00028 | 5 | 1 |
| 2 | 0.03491 | 0.03333 | 0.00058 | 0.00056 | 10 | 2 |
| 3 | 0.05236 | 0.05000 | 0.00087 | 0.00083 | 14 | 3 |
| 4 | 0.06981 | 0.06667 | 0.00116 | 0.00111 | 19 | 4 |
| 5 | 0.08727 | 0.08333 | 0.00145 | 0.00139 | 24 | 5 |
| 6 | 0.10472 | 0.10000 | 0.00175 | 0.00167 | 29 | 6 |
| 7 | 0.12217 | 0.11667 | 0.00204 | 0.00194 | 34 | 7 |
| 8 | 0.13963 | 0.13333 | 0.00233 | 0.00222 | 39 | 8 |
| 9 | 0.15708 | 0.15000 | 0.00262 | 0.00250 | 44 | 9 |
| 10 | 0.17453 | 0.16667 | 0.00291 | 0.00278 | 48 | 10 |
| 11 | 0.19199 | 0.18333 | 0.00320 | 0.00306 | 53 | 11 |
| 12 | 0.20944 | 0.20000 | 0.00349 | 0.00333 | 58 | 12 |
| 13 | 0.22689 | 0.21667 | 0.00378 | 0.00361 | 63 | 13 |
| 14 | 0.24435 | 0.23333 | 0.00407 | 0.00389 | 68 | 14 |
| 15 | 0.26180 | 0.25000 | 0.00436 | 0.00417 | 73 | 15 |
| 16 | 0.27925 | 0.26667 | 0.00465 | 0.00444 | 78 | 16 |
| 17 | 0.29671 | 0.28333 | 0.00495 | 0.00472 | 82 | 17 |
| 18 | 0.31416 | 0.30000 | 0.00524 | 0.00500 | 87 | 18 |
| 19 | 0.33161 | 0.31667 | 0.00553 | 0.00528 | 92 | 19 |
| 20 | 0.34907 | 0.33333 | 0.00582 | 0.00556 | 97 | 20 |
| 21 | 0.36652 | 0.35000 | 0.00611 | 0.00583 | 102 | 21 |
| 22 | 0.38397 | 0.36667 | 0.00640 | 0.00611 | 107 | 22 |
| 23 | 0.40143 | 0.38333 | 0.00669 | 0.00639 | 112 | 23 |
| 24 | 0.41888 | 0.40000 | 0.00698 | 0.00667 | 116 | 24 |
| 25 | 0.43633 | 0.41667 | 0.00727 | 0.00694 | 121 | 25 |
| 26 | 0.45379 | 0.43333 | 0.00756 | 0.00722 | 126 | 26 |
| 27 | 0.47124 | 0.45000 | 0.00785 | 0.00750 | 131 | 27 |
| 28 | 0.48869 | 0.46667 | 0.00814 | 0.00778 | 136 | 28 |
| 29 | 0.50615 | 0.48333 | 0.00844 | 0.00806 | 141 | 29 |
| 30 | 0.52360 | 0.50000 | 0.00873 | 0.00833 | 145 | 30 |
| 31 | 0.54105 | 0.51667 | 0.00902 | 0.00861 | 150 | 31 |
| 32 | 0.55851 | 0.53333 | 0.00931 | 0.00889 | 155 | 32 |
| 33 | 0.57596 | 0.55000 | 0.00960 | 0.00917 | 160 | 33 |
| 34 | 0.59341 | 0.56667 | 0.00989 | 0.00944 | 165 | 34 |
| 35 | 0.61087 | 0.58333 | 0.01018 | 0.00972 | 170 | 35 |
| 36 | 0.62832 | 0.60000 | 0.01047 | 0.01000 | 175 | 36 |
| 37 | 0.64577 | 0.61667 | 0.01076 | 0.01028 | 179 | 37 |
| 38 | 0.66323 | 0.63333 | 0.01105 | 0.01056 | 184 | 38 |
| 39 | 0.68068 | 0.65000 | 0.01134 | 0.01083 | 189 | 39 |
| 40 | 0.69813 | 0.66667 | 0.01164 | 0.01111 | 194 | 40 |

PROPORTIONAL PARTS

| | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 | 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 |
|---|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| 1 | 1.1 | 1.2 | 1.3 | 1.4 | 1.5 | 1.6 | 1.7 | 1.8 | 1.9 | 2.0 | 2.1 | 2.2 | 2.3 | 2.4 | 2.5 | 2.6 | 2.7 | 2.8 |
| 2 | 2.2 | 2.4 | 2.6 | 2.8 | 3.0 | 3.2 | 3.4 | 3.6 | 3.8 | 4.0 | 4.2 | 4.4 | 4.6 | 4.8 | 5.0 | 5.2 | 5.4 | 5.6 |
| 3 | 3.3 | 3.6 | 3.9 | 4.2 | 4.5 | 4.8 | 5.1 | 5.4 | 5.7 | 6.0 | 6.3 | 6.6 | 6.9 | 7.2 | 7.5 | 7.8 | 8.1 | 8.4 |
| 4 | 4.4 | 4.8 | 5.2 | 5.6 | 6.0 | 6.4 | 6.8 | 7.2 | 7.6 | 8.0 | 8.4 | 8.8 | 9.2 | 9.6 | 10.0 | 10.4 | 10.8 | 11.2 |
| 5 | 5.5 | 6.0 | 6.5 | 7.0 | 7.5 | 8.0 | 8.5 | 9.0 | 9.5 | 10.0 | 10.5 | 11.0 | 11.5 | 12.0 | 12.5 | 13.0 | 13.5 | 14.0 |
| 6 | 6.6 | 7.2 | 7.8 | 8.4 | 9.0 | 9.6 | 10.2 | 10.8 | 11.4 | 12.0 | 12.6 | 13.2 | 13.8 | 14.4 | 15.0 | 15.6 | 16.2 | 16.8 |
| 7 | 7.7 | 8.4 | 9.1 | 9.8 | 10.5 | 11.2 | 11.9 | 12.6 | 13.3 | 14.0 | 14.7 | 15.4 | 16.1 | 16.8 | 17.5 | 18.2 | 18.9 | 19.6 |
| 8 | 8.8 | 9.6 | 10.4 | 11.2 | 12.0 | 12.8 | 13.6 | 14.4 | 15.2 | 16.0 | 16.8 | 17.6 | 18.4 | 19.2 | 20.0 | 20.8 | 21.6 | 22.4 |
| 9 | 9.9 | 10.8 | 11.7 | 12.6 | 13.5 | 14.4 | 15.3 | 16.2 | 17.1 | 18.0 | 18.9 | 19.8 | 20.7 | 21.6 | 22.5 | 23.4 | 24.3 | 25.2 |
| | 29 | 30 | 31 | 32 | 33 | 34 | 35 | 36 | 37 | 38 | 39 | 40 | 41 | 42 | 43 | 44 | 45 | 46 |
| 1 | 2.9 | 3.0 | 3.1 | 3.2 | 3.3 | 3.4 | 3.5 | 3.6 | 3.7 | 3.8 | 3.9 | 4.0 | 4.1 | 4.2 | 4.3 | 4.4 | 4.5 | 4.6 |
| 2 | 5.8 | 6.0 | 6.2 | 6.4 | 6.6 | 6.8 | 7.0 | 7.2 | 7.4 | 7.6 | 7.8 | 8.0 | 8.2 | 8.4 | 8.6 | 8.8 | 9.0 | 9.2 |
| 3 | 8.7 | 9.0 | 9.3 | 9.6 | 9.9 | 10.2 | 10.5 | 10.8 | 11.1 | 11.4 | 11.7 | 12.0 | 12.3 | 12.6 | 12.9 | 13.2 | 13.5 | 13.8 |
| 4 | 11.6 | 12.0 | 12.4 | 12.8 | 13.2 | 13.6 | 14.0 | 14.4 | 14.8 | 15.2 | 15.6 | 16.0 | 16.4 | 16.8 | 17.2 | 17.6 | 18.0 | 18.4 |
| 5 | 14.5 | 15.0 | 15.5 | 16.0 | 16.5 | 17.0 | 17.5 | 18.0 | 18.5 | 19.0 | 19.5 | 20.0 | 20.5 | 21.0 | 21.5 | 22.0 | 22.5 | 23.0 |
| 6 | 17.4 | 18.0 | 18.6 | 19.2 | 19.8 | 20.4 | 21.0 | 21.6 | 22.2 | 22.8 | 23.4 | 24.0 | 24.6 | 25.2 | 25.8 | 26.4 | 27.0 | 27.6 |
| 7 | 20.3 | 21.0 | 21.7 | 22.4 | 23.1 | 23.8 | 24.5 | 25.2 | 25.9 | 26.6 | 27.3 | 28.0 | 28.7 | 29.4 | 30.1 | 30.8 | 31.5 | 32.2 |
| 8 | 23.2 | 24.0 | 24.8 | 25.6 | 26.4 | 27.2 | 28.0 | 28.8 | 29.6 | 30.4 | 31.2 | 32.0 | 32.8 | 33.6 | 34.4 | 35.2 | 36.0 | 36.8 |
| 9 | 26.1 | 27.0 | 27.9 | 28.8 | 29.7 | 30.6 | 31.5 | 32.4 | 33.3 | 34.2 | 35.1 | 36.0 | 36.9 | 37.8 | 38.7 | 39.6 | 40.5 | 41.4 |
| | 47 | 48 | 49 | 50 | 51 | 52 | 53 | 54 | 55 | 56 | 57 | 58 | 59 | 60 | 61 | 62 | 63 | 64 |
| 1 | 4.7 | 4.8 | 4.9 | 5.0 | 5.1 | 5.2 | 5.3 | 5.4 | 5.5 | 5.6 | 5.7 | 5.8 | 5.9 | 6.0 | 6.1 | 6.2 | 6.3 | 6.4 |
| 2 | 9.4 | 9.6 | 9.8 | 10.0 | 10.2 | 10.4 | 10.6 | 10.8 | 11.0 | 11.2 | 11.4 | 11.6 | 11.8 | 12.0 | 12.2 | 12.4 | 12.6 | 12.8 |
| 3 | 14.1 | 14.4 | 14.7 | 15.0 | 15.3 | 15.6 | 15.9 | 16.2 | 16.5 | 16.8 | 17.1 | 17.4 | 17.7 | 18.0 | 18.3 | 18.6 | 18.9 | 19.2 |
| 4 | 18.8 | 19.2 | 19.6 | 20.0 | 20.4 | 20.8 | 21.2 | 21.6 | 22.0 | 22.4 | 22.8 | 23.2 | 23.6 | 24.0 | 24.4 | 24.8 | 25.2 | 25.6 |
| 5 | 23.5 | 24.0 | 24.5 | 25.0 | 25.5 | 26.0 | 26.5 | 27.0 | 27.5 | 28.0 | 28.5 | 29.0 | 29.5 | 30.0 | 30.5 | 31.0 | 31.5 | 32.0 |
| 6 | 28.2 | 28.8 | 29.4 | 30.0 | 30.6 | 31.2 | 31.8 | 32.4 | 33.0 | 33.6 | 34.2 | 34.8 | 35.4 | 36.0 | 36.6 | 37.2 | 37.8 | 38.4 |
| 7 | 32.9 | 33.6 | 34.3 | 35.0 | 35.7 | 36.4 | 37.1 | 37.8 | 38.5 | 39.2 | 39.9 | 40.6 | 41.3 | 42.0 | 42.7 | 43.4 | 44.1 | 44.8 |
| 8 | 37.6 | 38.4 | 39.2 | 40.0 | 40.8 | 41.6 | 42.4 | 43.2 | 44.0 | 44.8 | 45.6 | 46.4 | 47.2 | 48.0 | 48.8 | 49.6 | 50.4 | 51.2 |
| 9 | 42.3 | 43.2 | 44.1 | 45.0 | 45.9 | 46.8 | 47.7 | 48.6 | 49.5 | 50.4 | 51.3 | 52.2 | 53.1 | 54.0 | 54.9 | 55.8 | 56.7 | 57.6 |
| | 65 | 66 | 67 | 68 | 69 | 70 | 71 | 72 | 73 | 74 | 75 | 76 | 77 | 78 | 79 | 80 | 81 | 82 |
| 1 | 6.5 | 6.6 | 6.7 | 6.8 | 6.9 | 7.0 | 7.1 | 7.2 | 7.3 | 7.4 | 7.5 | 7.6 | 7.7 | 7.8 | 7.9 | 8.0 | 8.1 | 8.2 |
| 2 | 13.0 | 13.2 | 13.4 | 13.6 | 13.8 | 14.0 | 14.2 | 14.4 | 14.6 | 14.8 | 15.0 | 15.2 | 15.4 | 15.6 | 15.8 | 16.0 | 16.2 | 16.4 |
| 3 | 19.5 | 19.8 | 20.1 | 20.4 | 20.7 | 21.0 | 21.3 | 21.6 | 21.9 | 22.2 | 22.5 | 22.8 | 23.1 | 23.4 | 23.7 | 24.0 | 24.3 | 24.6 |
| 4 | 26.0 | 26.4 | 26.8 | 27.2 | 27.6 | 28.0 | 28.4 | 28.8 | 29.2 | 29.6 | 30.0 | 30.4 | 30.8 | 31.2 | 31.6 | 32.0 | 32.4 | 32.8 |
| 5 | 32.5 | 33.0 | 33.5 | 34.0 | 34.5 | 35.0 | 35.5 | 36.0 | 36.5 | 37.0 | 37.5 | 38.0 | 38.5 | 39.0 | 39.5 | 40.0 | 40.5 | 41.0 |
| 6 | 39.0 | 39.6 | 40.2 | 40.8 | 41.4 | 42.0 | 42.6 | 43.2 | 43.8 | 44.4 | 45.0 | 45.6 | 46.2 | 46.8 | 47.4 | 48.0 | 48.6 | 49.2 |
| 7 | 45.5 | 46.2 | 46.9 | 47.6 | 48.3 | 49.0 | 49.7 | 50.4 | 51.1 | 51.8 | 52.5 | 53.2 | 53.9 | 54.6 | 55.3 | 56.0 | 56.7 | 57.4 |
| 8 | 52.0 | 52.8 | 53.6 | 54.4 | 55.2 | 56.0 | 56.8 | 57.6 | 58.4 | 59.2 | 60.0 | 60.8 | 61.6 | 62.4 | 63.2 | 64.0 | 64.8 | 65.6 |
| 9 | 58.5 | 59.4 | 60.3 | 61.2 | 62.1 | 63.0 | 63.9 | 64.8 | 65.7 | 66.6 | 67.5 | 68.4 | 69.3 | 70.2 | 71.1 | 72.0 | 72.9 | 73.8 |
| | 83 | 84 | 85 | 86 | 87 | 88 | 89 | 90 | 91 | 92 | 93 | 94 | 95 | 96 | 97 | 98 | 99 | 100 |
| 1 | 8.3 | 8.4 | 8.5 | 8.6 | 8.7 | 8.8 | 8.9 | 9.0 | 9.1 | 9.2 | 9.3 | 9.4 | 9.5 | 9.6 | 9.7 | 9.8 | 9.9 | 10.0 |
| 2 | 16.6 | 16.8 | 17.0 | 17.2 | 17.4 | 17.6 | 17.8 | 18.0 | 18.2 | 18.4 | 18.6 | 18.8 | 19.0 | 19.2 | 19.4 | 19.6 | 19.8 | 20.0 |
| 3 | 24.9 | 25.2 | 25.5 | 25.8 | 26.1 | 26.4 | 26.7 | 27.0 | 27.3 | 27.6 | 27.9 | 28.2 | 28.5 | 28.8 | 29.1 | 29.4 | 29.7 | 30.0 |
| 4 | 33.2 | 33.6 | 34.0 | 34.4 | 34.8 | 35.2 | 35.6 | 36.0 | 36.4 | 36.8 | 37.2 | 37.6 | 38.0 | 38.4 | 38.8 | 39.2 | 39.6 | 40.0 |
| 5 | 41.5 | 42.0 | 42.5 | 43.0 | 43.5 | 44.0 | 44.5 | 45.0 | 45.5 | 46.0 | 46.5 | 47.0 | 47.5 | 48.0 | 48.5 | 49.0 | 49.5 | 50.0 |
| 6 | 49.8 | 50.4 | 51.0 | 51.6 | 52.2 | 52.8 | 53.4 | 54.0 | 54.6 | 55.2 | 55.8 | 56.4 | 57.0 | 57.6 | 58.2 | 58.8 | 59.4 | 60.0 |
| 7 | 58.1 | 58.8 | 59.5 | 60.2 | 60.9 | 61.6 | 62.3 | 63.0 | 63.7 | 64.4 | 65.1 | 65.8 | 66.5 | 67.2 | 67.9 | 68.6 | 69.3 | 70.0 |
| 8 | 66.4 | 67.2 | 68.0 | 68.8 | 69.6 | 70.4 | 71.2 | 72.0 | 72.8 | 73.6 | 74.4 | 75.2 | 76.0 | 76.8 | 77.6 | 78.4 | 79.2 | 80.0 |
| 9 | 74.7 | 75.6 | 76.5 | 77.4 | 78.3 | 79.2 | 80.1 | 81.0 | 81.9 | 82.8 | 83.7 | 84.6 | 85.5 | 86.4 | 87.3 | 88.2 | 89.1 | 90.0 |

PROPORTIONAL PARTS

| | 101 | 102 | 103 | 104 | 105 | 106 | 107 | 108 | 109 | 110 | 111 | 112 | 113 | 114 | 115 |
|---|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| 1 | 10.1 | 10.2 | 10.3 | 10.4 | 10.5 | 10.6 | 10.7 | 10.8 | 10.9 | 11.0 | 11.1 | 11.2 | 11.3 | 11.4 | 11.5 |
| 2 | 20.2 | 20.4 | 20.6 | 20.8 | 21.0 | 21.2 | 21.4 | 21.6 | 21.8 | 22.0 | 22.2 | 22.4 | 22.6 | 22.8 | 23.0 |
| 3 | 30.3 | 30.6 | 30.9 | 31.2 | 31.5 | 31.8 | 32.1 | 32.4 | 32.7 | 33.0 | 33.3 | 33.6 | 33.9 | 34.2 | 34.5 |
| 4 | 40.4 | 40.8 | 41.2 | 41.6 | 42.0 | 42.4 | 42.8 | 43.2 | 43.6 | 44.0 | 44.4 | 44.8 | 45.2 | 45.6 | 46.0 |
| 5 | 50.5 | 51.0 | 51.5 | 52.0 | 52.5 | 53.0 | 53.5 | 54.0 | 54.5 | 55.0 | 55.5 | 56.0 | 56.5 | 57.0 | 57.5 |
| 6 | 60.6 | 61.2 | 61.8 | 62.4 | 63.0 | 63.6 | 64.2 | 64.8 | 65.4 | 66.0 | 66.6 | 67.2 | 67.8 | 68.4 | 69.0 |
| 7 | 70.7 | 71.4 | 72.1 | 72.8 | 73.5 | 74.2 | 74.9 | 75.6 | 76.3 | 77.0 | 77.7 | 78.4 | 79.1 | 79.8 | 80.5 |
| 8 | 80.8 | 81.6 | 82.4 | 83.2 | 84.0 | 84.8 | 85.6 | 86.4 | 87.2 | 88.0 | 88.8 | 89.6 | 90.4 | 91.2 | 92.0 |
| 9 | 90.9 | 91.8 | 92.7 | 93.6 | 94.5 | 95.4 | 96.3 | 97.2 | 98.1 | 99.0 | 99.9 | 100.8 | 101.7 | 102.6 | 103.5 |
| | 116 | 117 | 118 | 119 | 120 | 121 | 122 | 123 | 124 | 125 | 126 | 127 | 128 | 129 | 130 |
| 1 | 11.6 | 11.7 | 11.8 | 11.9 | 12.0 | 12.1 | 12.2 | 12.3 | 12.4 | 12.5 | 12.6 | 12.7 | 12.8 | 12.9 | 13.0 |
| 2 | 23.2 | 23.4 | 23.6 | 23.8 | 24.0 | 24.2 | 24.4 | 24.6 | 24.8 | 25.0 | 25.2 | 25.4 | 25.6 | 25.8 | 26.0 |
| 3 | 34.8 | 35.1 | 35.4 | 35.7 | 36.0 | 36.3 | 36.6 | 36.9 | 37.2 | 37.5 | 37.8 | 38.1 | 38.4 | 38.7 | 39.0 |
| 4 | 46.4 | 46.8 | 47.2 | 47.6 | 48.0 | 48.4 | 48.8 | 49.2 | 49.6 | 50.0 | 50.4 | 50.8 | 51.2 | 51.6 | 52.0 |
| 5 | 58.0 | 58.5 | 59.0 | 59.5 | 60.0 | 60.5 | 61.0 | 61.5 | 62.0 | 62.5 | 63.0 | 63.5 | 64.0 | 64.5 | 65.0 |
| 6 | 69.6 | 70.2 | 70.8 | 71.4 | 72.0 | 72.6 | 73.2 | 73.8 | 74.4 | 75.0 | 75.6 | 76.2 | 76.8 | 77.4 | 78.0 |
| 7 | 81.2 | 81.9 | 82.6 | 83.3 | 84.0 | 84.7 | 85.4 | 86.1 | 86.8 | 87.5 | 88.2 | 88.9 | 89.6 | 90.3 | 91.0 |
| 8 | 92.8 | 93.6 | 94.4 | 95.2 | 96.0 | 96.8 | 97.6 | 98.4 | 99.2 | 100.0 | 100.8 | 101.6 | 102.4 | 103.2 | 104.0 |
| 9 | 104.4 | 105.3 | 106.2 | 107.1 | 108.0 | 108.9 | 109.8 | 110.7 | 111.6 | 112.5 | 113.4 | 114.3 | 115.2 | 116.1 | 117.0 |
| | 131 | 132 | 133 | 134 | 135 | 136 | 137 | 138 | 139 | 140 | 141 | 142 | 143 | 144 | 145 |
| 1 | 13.1 | 13.2 | 13.3 | 13.4 | 13.5 | 13.6 | 13.7 | 13.8 | 13.9 | 14.0 | 14.1 | 14.2 | 14.3 | 14.4 | 14.5 |
| 2 | 26.2 | 26.4 | 26.6 | 26.8 | 27.0 | 27.2 | 27.4 | 27.6 | 27.8 | 28.0 | 28.2 | 28.4 | 28.6 | 28.8 | 29.0 |
| 3 | 39.3 | 39.6 | 39.9 | 40.2 | 40.5 | 40.8 | 41.1 | 41.4 | 41.7 | 42.0 | 42.3 | 42.6 | 42.9 | 43.2 | 43.5 |
| 4 | 52.4 | 52.8 | 53.2 | 53.6 | 54.0 | 54.4 | 54.8 | 55.2 | 55.6 | 56.0 | 56.4 | 56.8 | 57.2 | 57.6 | 58.0 |
| 5 | 65.5 | 66.0 | 66.5 | 67.0 | 67.5 | 68.0 | 68.5 | 69.0 | 69.5 | 70.0 | 70.5 | 71.0 | 71.5 | 72.0 | 72.5 |
| 6 | 78.6 | 79.2 | 79.8 | 80.4 | 81.0 | 81.6 | 82.2 | 82.8 | 83.4 | 84.0 | 84.6 | 85.2 | 85.8 | 86.4 | 87.0 |
| 7 | 91.7 | 92.4 | 93.1 | 93.8 | 94.5 | 95.2 | 95.9 | 96.6 | 97.3 | 98.0 | 98.7 | 99.4 | 100.1 | 100.8 | 101.5 |
| 8 | 104.8 | 105.6 | 106.4 | 107.2 | 108.0 | 108.8 | 109.6 | 110.4 | 111.2 | 112.0 | 112.8 | 113.6 | 114.4 | 115.2 | 116.0 |
| 9 | 117.9 | 118.8 | 119.7 | 120.6 | 121.5 | 122.4 | 123.3 | 124.2 | 125.1 | 126.0 | 126.9 | 127.8 | 128.7 | 129.6 | 130.5 |
| | 146 | 147 | 148 | 149 | 150 | 151 | 152 | 153 | 154 | 155 | 156 | 157 | 158 | 159 | 160 |
| 1 | 14.6 | 14.7 | 14.8 | 14.9 | 15.0 | 15.1 | 15.2 | 15.3 | 15.4 | 15.5 | 15.6 | 15.7 | 15.8 | 15.9 | 16.0 |
| 2 | 29.2 | 29.4 | 29.6 | 29.8 | 30.0 | 30.2 | 30.4 | 30.6 | 30.8 | 31.0 | 31.2 | 31.4 | 31.6 | 31.8 | 32.0 |
| 3 | 43.8 | 44.1 | 44.4 | 44.7 | 45.0 | 45.3 | 45.6 | 45.9 | 46.2 | 46.5 | 46.8 | 47.1 | 47.4 | 47.7 | 48.0 |
| 4 | 58.4 | 58.8 | 59.2 | 59.6 | 60.0 | 60.4 | 60.8 | 61.2 | 61.6 | 62.0 | 62.4 | 62.8 | 63.2 | 63.6 | 64.0 |
| 5 | 73.0 | 73.5 | 74.0 | 74.5 | 75.0 | 75.5 | 76.0 | 76.5 | 77.0 | 77.5 | 78.0 | 78.5 | 79.0 | 79.5 | 80.0 |
| 6 | 87.6 | 88.2 | 88.8 | 89.4 | 90.0 | 90.6 | 91.2 | 91.8 | 92.4 | 93.0 | 93.6 | 94.2 | 94.8 | 95.4 | 96.0 |
| 7 | 102.2 | 102.9 | 103.6 | 104.3 | 105.0 | 105.7 | 106.4 | 107.1 | 107.8 | 108.5 | 109.2 | 109.9 | 110.6 | 111.3 | 112.0 |
| 8 | 116.8 | 117.6 | 118.4 | 119.2 | 120.0 | 120.8 | 121.6 | 122.4 | 123.2 | 124.0 | 124.8 | 125.6 | 126.4 | 127.2 | 128.0 |
| 9 | 131.4 | 132.3 | 133.2 | 134.1 | 135.0 | 135.9 | 136.8 | 137.7 | 138.6 | 139.5 | 140.4 | 141.3 | 142.2 | 143.1 | 144.0 |
| | 161 | 162 | 163 | 164 | 165 | 166 | 167 | 168 | 169 | 170 | 171 | 172 | 173 | 174 | 175 |
| 1 | 16.1 | 16.2 | 16.3 | 16.4 | 16.5 | 16.6 | 16.7 | 16.8 | 16.9 | 17.0 | 17.1 | 17.2 | 17.3 | 17.4 | 17.5 |
| 2 | 32.2 | 32.4 | 32.6 | 32.8 | 33.0 | 33.2 | 33.4 | 33.6 | 33.8 | 34.0 | 34.2 | 34.4 | 34.6 | 34.8 | 35.0 |
| 3 | 48.3 | 48.6 | 48.9 | 49.2 | 49.5 | 49.8 | 50.1 | 50.4 | 50.7 | 51.0 | 51.3 | 51.6 | 51.9 | 52.2 | 52.5 |
| 4 | 64.4 | 64.8 | 65.2 | 65.6 | 66.0 | 66.4 | 66.8 | 67.2 | 67.6 | 68.0 | 68.4 | 68.8 | 69.2 | 69.6 | 70.0 |
| 5 | 80.5 | 81.0 | 81.5 | 82.0 | 82.5 | 83.0 | 83.5 | 84.0 | 84.5 | 85.0 | 85.5 | 86.0 | 86.5 | 87.0 | 87.5 |
| 6 | 96.6 | 97.2 | 97.8 | 98.4 | 99.0 | 99.6 | 100.2 | 100.8 | 101.4 | 102.0 | 102.6 | 103.2 | 103.8 | 104.4 | 105.0 |
| 7 | 112.7 | 113.4 | 113.1 | 114.8 | 115.5 | 116.2 | 116.9 | 117.6 | 118.3 | 119.0 | 119.7 | 120.4 | 121.1 | 121.8 | 122.5 |
| 8 | 128.8 | 129.6 | 130.4 | 131.2 | 132.0 | 132.8 | 133.6 | 134.4 | 135.2 | 136.0 | 136.8 | 137.6 | 138.4 | 139.2 | 140.0 |
| 9 | 144.9 | 145.8 | 146.7 | 147.6 | 148.5 | 149.4 | 150.3 | 151.2 | 152.1 | 153.0 | 153.9 | 154.8 | 155.7 | 156.6 | 157.5 |

8.6. CONVERSIONS OF DEGREES TO RADIANS, ETC.

TABLE 8.6 (continued)

| No. of
degrees,
minutes
or seconds | Degrees in
radians | Minutes in
decimals of
degree | Minutes in
radians | Seconds in
decimals of
degree | Seconds in
radians
× 10 ⁶ | No. |
|---|-----------------------|-------------------------------------|-----------------------|-------------------------------------|--|-----|
| 41 | 0.71558 | 0.68333 | 0.01193 | 0.01139 | 199 | 41 |
| 42 | 0.73304 | 0.70000 | 0.01222 | 0.01167 | 204 | 42 |
| 43 | 0.75049 | 0.71667 | 0.01251 | 0.01194 | 208 | 43 |
| 44 | 0.76794 | 0.73333 | 0.01280 | 0.01222 | 213 | 44 |
| 45 | 0.78540 | 0.75000 | 0.01309 | 0.01250 | 218 | 45 |
| 46 | 0.80285 | 0.76667 | 0.01338 | 0.01278 | 223 | 46 |
| 47 | 0.82030 | 0.78333 | 0.01367 | 0.01306 | 228 | 47 |
| 48 | 0.83776 | 0.80000 | 0.01396 | 0.01333 | 233 | 48 |
| 49 | 0.85521 | 0.81667 | 0.01425 | 0.01361 | 238 | 49 |
| 50 | 0.87266 | 0.83333 | 0.01454 | 0.01389 | 242 | 50 |
| 51 | 0.89012 | 0.85000 | 0.01484 | 0.01417 | 247 | 51 |
| 52 | 0.90757 | 0.86667 | 0.01513 | 0.01444 | 252 | 52 |
| 53 | 0.92502 | 0.88333 | 0.01542 | 0.01472 | 257 | 53 |
| 54 | 0.94248 | 0.90000 | 0.01571 | 0.01500 | 262 | 54 |
| 55 | 0.95993 | 0.91667 | 0.01600 | 0.01528 | 267 | 55 |
| 56 | 0.97738 | 0.93333 | 0.01629 | 0.01556 | 272 | 56 |
| 57 | 0.99484 | 0.95000 | 0.01658 | 0.01583 | 276 | 57 |
| 58 | 1.01229 | 0.96667 | 0.01687 | 0.01611 | 281 | 58 |
| 59 | 1.02974 | 0.98333 | 0.01716 | 0.01639 | 286 | 59 |
| 60 | 1.04720 | 1.00000 | 0.01745 | 0.01667 | 291 | 60 |

| Degrees | Radians | Degrees | Radians | Degrees | Radians | Degrees | Radians |
|---------|---------|---------|---------|---------|----------|---------|-------------------|
| 61 | 1.06465 | 81 | 1.41372 | 200 | 3.49066 | 180 | π 3.14159 |
| 62 | 1.08210 | 82 | 1.43117 | 300 | 5.23599 | 270 | 1.5π 4.71239 |
| 63 | 1.09956 | 83 | 1.44862 | 400 | 6.98132 | 360 | 2π 6.28319 |
| 64 | 1.11701 | 84 | 1.46608 | 500 | 8.72665 | 450 | 2.5π 7.85398 |
| 65 | 1.13446 | 85 | 1.48353 | 600 | 10.47198 | 540 | 3π 9.42478 |
| 66 | 1.15192 | 86 | 1.50098 | 700 | 12.21730 | 630 | 3.5π 10.99557 |
| 67 | 1.16937 | 87 | 1.51844 | 800 | 13.96263 | 720 | 4π 12.56637 |
| 68 | 1.18682 | 88 | 1.53589 | 900 | 15.70796 | 810 | 4.5π 14.13717 |
| 69 | 1.20428 | 89 | 1.55334 | 1000 | 17.45329 | 900 | 5π 15.70796 |
| 70 | 1.22173 | 90 | 1.57080 | 1100 | 19.19862 | 990 | 5.5π 17.27876 |
| 71 | 1.23918 | 91 | 1.58825 | 1200 | 20.94395 | 1080 | 6π 18.84956 |
| 72 | 1.25664 | 92 | 1.60570 | 1300 | 22.68928 | 1170 | 6.5π 20.42035 |
| 73 | 1.27409 | 93 | 1.62316 | 1400 | 24.43461 | 1260 | 7π 21.99115 |
| 74 | 1.29154 | 94 | 1.64061 | 1500 | 26.17994 | 1350 | 7.5π 23.56194 |
| 75 | 1.30900 | 95 | 1.65806 | 1600 | 27.92526 | 1440 | 8π 25.13274 |
| 76 | 1.32645 | 96 | 1.67552 | 1700 | 29.67059 | 1530 | 8.5π 26.70354 |
| 77 | 1.34390 | 97 | 1.69297 | 1800 | 31.41593 | 1620 | 9π 28.27433 |
| 78 | 1.36136 | 98 | 1.71042 | 1900 | 33.16126 | 1710 | 9.5π 29.84512 |
| 79 | 1.37881 | 99 | 1.72788 | 2000 | 34.90659 | 1800 | 10π 31.41593 |
| 80 | 1.39626 | 100 | 1.74533 | | | | |

TABLE 8.6 (continued)

| Degrees | | Radians | Degrees | | Radians | Degrees | | Radians |
|---------|------|----------|---------|-----------|----------|---------|------|----------|
| Dec. | Min. | | Dec. | Min. Sec. | | Dec. | Sec. | |
| 0.1 | 6 | 0.001745 | 0.01 | 0 36 | 0.000174 | 0.001 | 3.6 | 0.000017 |
| 0.2 | 12 | 0.003491 | 0.02 | 1 12 | 0.000349 | 0.002 | 7.2 | 0.000035 |
| 0.3 | 18 | 0.005236 | 0.03 | 1 48 | 0.000524 | 0.003 | 10.8 | 0.000052 |
| 0.4 | 24 | 0.006981 | 0.04 | 2 24 | 0.000698 | 0.004 | 14.4 | 0.000070 |
| 0.5 | 30 | 0.008727 | 0.05 | 3 0 | 0.000873 | 0.005 | 18.0 | 0.000087 |
| 0.6 | 36 | 0.010472 | 0.06 | 3 36 | 0.001047 | 0.006 | 21.6 | 0.000105 |
| 0.7 | 42 | 0.012217 | 0.07 | 4 12 | 0.001222 | 0.007 | 25.2 | 0.000122 |
| 0.8 | 48 | 0.013963 | 0.08 | 4 48 | 0.001396 | 0.008 | 28.8 | 0.000140 |
| 0.9 | 54 | 0.015708 | 0.09 | 5 24 | 0.001571 | 0.009 | 32.4 | 0.000157 |

| Rad. | Deg. | Rad. | Deg. | Rad. | Deg. | Rad. | Deg. | Rad. | Deg. |
|------|----------|------|---------|------|--------|-------|--------|--------|--------|
| 1 | 57.2958 | 0.1 | 5.7296 | 0.01 | 0.5730 | 0.001 | 0.0573 | 0.0001 | 0.0057 |
| 2 | 114.5916 | 0.2 | 11.4592 | 0.02 | 1.1459 | 0.002 | 0.1146 | 0.0002 | 0.0115 |
| 3 | 171.8873 | 0.3 | 17.1887 | 0.03 | 1.7189 | 0.003 | 0.1719 | 0.0003 | 0.0172 |
| 4 | 229.1831 | 0.4 | 22.9183 | 0.04 | 2.2918 | 0.004 | 0.2292 | 0.0004 | 0.0229 |
| 5 | 286.4789 | 0.5 | 28.6479 | 0.05 | 2.8648 | 0.005 | 0.2865 | 0.0005 | 0.0286 |
| 6 | 343.7747 | 0.6 | 34.3775 | 0.06 | 3.4378 | 0.006 | 0.3438 | 0.0006 | 0.0344 |
| 7 | 401.0705 | 0.7 | 40.1070 | 0.07 | 4.0107 | 0.007 | 0.4011 | 0.0007 | 0.0401 |
| 8 | 458.3662 | 0.8 | 45.8366 | 0.08 | 4.5837 | 0.008 | 0.4584 | 0.0008 | 0.0458 |
| 9 | 515.6620 | 0.9 | 51.5662 | 0.09 | 5.1566 | 0.009 | 0.5157 | 0.0009 | 0.0516 |

Section 9

DICTIONARY OF CRYSTALLOGRAPHIC TERMS FOR VOLUME II

**In English, French, German, Russian and Spanish,
together with the Greek and Russian Alphabets**

| | PAGE |
|--|------|
| 9.1. GREEK ALPHABET | 435 |
| 9.2. RUSSIAN ALPHABET | 435 |
| 9.3. DICTIONARY OF CRYSTALLOGRAPHIC TERMS IN ENGLISH, FRENCH, GERMAN, RUSSIAN
AND SPANISH (<i>J. L. Amorós, V. Balashov, M. L. Canut, G. Donnay, J. D. H. Donnay, P. P. Ewald,
N. F. M. Henry, F. Laves, A. L. Mackay, A. V. Rzhhanov, A. V. Shubnikov, A. V. Spitsin and others</i>) | 436 |
| 9.3.1. List of terms in English which are similar (or easily recognizable) in all the five languages .. | 436 |
| 9.3.2. List of terms which are similar (or easily recognizable) in English, French, German and
Spanish (English and Russian equivalents only are given) | 438 |
| 9.3.3. List of other English terms used in Volume II, with equivalents in French, German, Russian
and Spanish | 439 |

9.1. Greek Alphabet

| | | |
|-------------------------|----------------------------|-------------------------|
| A α alpha | I ι iota | P ρ rho |
| B β beta | K κ kappa | Σ σ sigma |
| Γ γ gamma | Λ λ lambda | T τ tau |
| Δ δ delta | M μ mu | Y υ upsilon |
| E ϵ epsilon | N ν nu | Φ ϕ phi |
| Z ζ zeta | Ξ ξ xi | X χ chi |
| H η eta | O o omicron | Ψ ψ psi |
| Θ θ theta | Π π pi | Ω ω omega |

9.2. Russian Alphabet

| | | <i>Sound as in</i> | | | <i>Sound as in</i> |
|---|----|--|---|---|--|
| А | а | arc (stressed)
<i>hexagon</i> (unstressed) | П | п | peak |
| Б | б | base | Р | р | ratio (strongly rolled) |
| В | в | vector | С | с | sign, cell |
| Г | г* | goniometer | Т | т | tensor |
| Д | д | dyad | У | у | group |
| Е | е | yellow | Ф | ф | film |
| Ё | ё | yon | Х | х | loch |
| Ж | ж | measure | Ц | ц | nets, quartz |
| З | з | zone | Ч | ч | chart |
| И | и | machine | Ш | ш | shape |
| Й | й | ray | Щ | щ | mesh chain |
| К | к | key; cone | Ъ | ъ | (or ') silent; denotes hard consonant preceding |
| Л | л | line | Ы | ы | pyramid |
| М | м | minus | Ь | ь | silent; denotes soft consonant preceding |
| Н | н | node | Э | э | net |
| О | о | odd (stressed)
error (unstressed) | Ю | ю | unit |
| | | | Я | я | yard |

* The letter Г r is often used where H h would occur in the English equivalent. There is no aspirate in the Russian alphabet.

9.3. Dictionary of Crystallographic Terms in English, French, German, Russian and Spanish

9.3.1. List of Terms in English which are similar (or easily recognizable) in all the Five Languages

| | | |
|------------------------|------------------------------|-----------------------------|
| Abelian group | cosine | Icosahedron |
| aberration | cotangent | identical |
| absolute configuration | covalent | identification |
| abstract group | covariance | index; indices |
| algebra | criterion | integral (calculus) |
| analogue (optical) | cubo-octahedron | integration |
| analysis | cycle; cyclic | intensity |
| analytical geometry | cylinder | interference |
| anisotropic | | interpolation |
| anomalous dispersion | | invariant |
| antisymmetric | | inverse; inversion |
| argument | Delta function | irrational |
| arithmetic | delta, Kronecker | isomorphous |
| aspect | determinant | isotropic |
| associative (rule) | diagonal form | iteration |
| azimuth | diagonalization | |
| | differentiation | |
| | diffraction | Linear |
| | duality | logarithm |
| | dyad | Lorentz factor |
| | | Lorentz-polarization factor |
| Bessel function | | |
| bibliography | | |
| binomial theorem | | |
| bivariate | | |
| | Eccentricity | Machine |
| | element | mantissa |
| | ellipse; ellipsoid | massive (specimen) |
| | enantiomorphous | matrix |
| | equatorial | maximum |
| Canonical form | extinction | median |
| Cartesian | Euclidean | meridian |
| central moment | extrapolation | Miller indices |
| centrosymmetry | | minimum |
| characteristic | | minor (of determinant) |
| class | | minus |
| coefficient | Formal (solution) | mnemonic |
| collimator | function | mode |
| collinear | | modulo |
| column | | modulus |
| commutative | | molecular transform |
| complex | Geometric | moment |
| concrete | gnomonic (net or projection) | monochromatic |
| cone | goniometer | monoclinic |
| configuration | group | morphology |
| congruent | | mosaic |
| contour | | |
| contravariance | | |
| convention | Harmonic | |
| coplanar | Hermite function; Hermitian | Napier's rules |
| co-ordinates | hexagon; hexagonal | natural (number, logarithm) |
| co-ordination | homogeneous | normal |
| correlation | homometric | normalize |
| cosecant | hyperbola; hyperboloid | null |

9.3. DICTIONARY OF CRYSTALLOGRAPHIC TERMS

| | | |
|--|----------------------------------|-----------------------------|
| Octahedron | progression | Tangent |
| octant | projection | temperature factor |
| operation | proportionality | tensor |
| optical isomers | | tetragonal |
| order (of determinant or spectrum) | | tetrahedral; tetrahedron |
| orientation | | texture |
| orthohexagonal | Quadrant | transcendental (equations) |
| orthorhombic | quadratic | transform |
| | quantum mechanics | transpose |
| | | triclinic (anorthic) |
| | | trigonal |
| | | trigonometry |
| | | trinomial |
| | | triplet |
| | | trivial (solution) |
| Parabola; paraboloid | Radian | |
| parallel | rational indices | |
| parallelogram | rhombohedral; rhombohedron | |
| parallelepiped | | |
| parameter | | |
| peak (maximum) | Scalar | |
| period; periodic | secant | Unitary structure amplitude |
| phase | sine | |
| photosommateur (G. v. Eller) | singular (matrix) | |
| polar (co-ordinates, direction) | sinusoidal | |
| polarization | special (case, position, vector) | Vector; vectorial |
| polarized (beam) | sphere | |
| pole | statistical; statistics | |
| polyhedron | steradian | |
| polynomial | stereogram | Wulff net |
| precession (camera, method) | structure factor | |
| prefactor | summation | |
| primitive (cell, translation, triplet) | synthesis | |
| programme (of computer) | system; systematic | Zone |

9.3. DICTIONARY OF CRYSTALLOGRAPHIC TERMS

9.3.2. List of terms which are similar (or easily recognizable) in English, French, German and Spanish (English and Russian equivalents only are given)

| ENGLISH | RUSSIAN | ENGLISH | RUSSIAN |
|--|--|--|--|
| Absorption
adjoint
approximations,
successive | поглощение
сопряженный
приближения,
последовательные | Multiplicity | многократность |
| Concave
conjugate

conjunction
convergent;
convergence
convex | вогнутый
сопрягать;
сопряженный
соединение
сходящийся;
сходимость
выпуклый | Negative (—)
numerical

Parity
particle
permutation
positive (+)
primary (extinction) | отрицательный
численный

четность
частица
перестановка
положительный
первичная (экстинкция) |
| Decimal
density, electron
difference synthesis
differential calculus

dimensions
direct (lattice, vector)

direction cosine
discontinuity
discrete values
divergent-beam method

divide; division | десятичный
электронная плотность
разностный синтез
дифференциальное
исчисление
размеры
решетка, вектор в
реальном пространстве
направляющий косинус
прерывность
дискретные величины
метод расходящегося
пучка
делить; деление | Quotient

Reciprocal
rectangular
reduced cell
reference | частное

обратный
прямоугольный
приведенная ячейка
ссылка |
| Elastic constants
eliminate
explicit | константы упругости
исключать
точный (определенный) | Secondary (extinction)
simultaneous
substitution
subtraction | вторичная (экстинкция)
одновременный
замещение, подстановка
вычитание |
| Festoon (Weissenberg)
frequency | гирлянда
частота | Transformation | преобразование |
| Idemfactor
imaginary
intermediate | единичная матрица
мнимый
промежуточный | Vertical divergence | вертикальное
расхождение |

9.3. DICTIONARY OF CRYSTALLOGRAPHIC TERMS

9.3.3. List of other English terms used, with equivalents in French, German, Russian and Spanish

| ENGLISH | FRENCH | GERMAN | RUSSIAN | SPANISH |
|------------------------------------|---|--|-------------------------------------|--|
| Abbreviation | abréviation | Abkürzung | сокращение | abreviación |
| absence | absence | Abwesenheit;
Auslöschung | отсутствие (погасание) | extinción; ausencia |
| absolute value | valeur absolue | absoluter Wert | абсолютная величина | valor absoluto |
| accuracy | exactitude; véracité | Genauigkeit | точность | exactitud |
| adding machine | machine à additionner | Addiermaschine;
Additionsmaschine | суммирующая машина | máquina sumadora |
| addition | addition | Addition | сложение | suma |
| adjacent | contigu | anliegend; benachbart | смежный;
прилегающий | adyacente |
| angle | angle | Winkel | угол | ángulo |
| anomalous scattering | diffusion anormale | anomale Streuung | аномальное рассеяние | difracción anómala |
| antecedent | antécédent | vorhergehend | предыдущий | antecedente |
| anti-equi-inclination | anti-équi-inclinaison | entgegengesetzte gleiche
Neigung | антиравное наклонение | anti-equi-inclinación |
| approximate | approximatif | annähernd | приближенный | aproximado |
| arbitrary | arbitraire | willkürlich | произвольный | arbitrario |
| arc | arc | Bogen | дуга | arco |
| auto-convolution | autocorrélation | Selbstfaltung | самосвертка
(самосвертывание) | autoconvolución |
| average | moyenne | Durchschnitt; Mittelwert | среднее | promedio |
| axis; axes | axe; axes | Achse; Achsen | ось; оси | eje; ejes |
| | | | | |
| Basic operation | opération fondamentale | Grundoperation;
Fundamentaloperation | основная операция | operación fundamental |
| binary computer | calculateur binaire;
calculateur à base deux | binäre Rechenmaschine | двоичная вычислительная машина | calculadora binaria |
| binomial theorem | binôme de Newton | binomischer Lehrsatz | биномиальная теорема | teorema del binomio |
| body diagonal | diagonale du cube,
du solide | Raumdiagonale;
Körperdiagonale | пространственная диагональ | diagonal espacial |
| bond angles | angles des liaisons | Bindungswinkel | углы между связями | ángulos de enlace |
| bond lengths | longueurs de liaison | Bindungslängen | длины связей | distancias de enlace |
| bound, lower | borne inférieure | untere Schranke | граница, нижняя | límite inferior |
| bound, upper | borne supérieure | obere Schranke | граница, верхняя | límite superior |
| bounded projection | projection limitée | begrenzte Projektion;
Schichtprojektion | поясная проекция | proyección limitada |
| breadth, line | largeur de la raie | Linienbreite | ширина, линии | anchura de la raya |
| breadth, half-value | largeur à mi-hauteur | Halbwertsbreite | полуширина | anchura media |
| | | | | |
| Calculation;
computation | calcul | Berechnung; Rechnung | вычисление | cálculo |
| calculating (computing)
machine | machine à calculer | Rechenmaschine | счетная машина | máquina de calcular |
| calculus, differential | calcul différentiel | Differentialrechnung | исчисление,
дифференциальное | cálculo diferencial |
| calculus, integral | calcul intégral | Integralrechnung | исчисление,
интегральное | cálculo integral |
| calibration | étalonnage | Kalibrierung; Eichung | калибровка | calibrado |
| cell | maille | Zelle; Elementarzelle | ячейка | celda |
| centre of gravity | centre de gravité | Schwerpunkt | центр тяжести | centro de gravedad |
| chart | abaque | Tafel; Diagramm;
Nomogramm | диаграмма; таблица;
номограмма | carta; cánvas; falsilla |
| chemical composition | composition chimique | chemische Zusammen-
setzung | химический состав | composición química |
| circumference | circonférence | Kreisumfang; Umfang | окружность
(окружение) | circunferencia |
| cleavage | clivage | Spaltbarkeit; Spaltung | спайность | exfoliación |
| close-packing | empilement compact;
assemblage compact | dichteste Packung | плотная упаковка | empaquetado denso |
| close-packing, cubic | assemblage compact
cubique | dichteste Packung,
kubische | плотная упаковка,
кубическая | empaquetado denso
cúbico; empaquetado
cúbico |
| close-packing, hexagonal | assemblage compact
sénaire | dichteste Packung,
hexagonale | плотная упаковка,
гексагональная | empaquetado hexagonal |

9.3. DICTIONARY OF CRYSTALLOGRAPHIC TERMS

| ENGLISH | FRENCH | GERMAN | RUSSIAN | SPANISH |
|---|---|---|---|---------------------------------------|
| column matrix | matrice forme colonne | einspaltige Matrix;
Kolonnenmatrix | столбчатая матрица | matriz de una columna |
| commute | commuter | vertauschen | перестановлять | commutar |
| component | composante | Bestandteil; Komponente | компонента
(составляющая) | componente |
| condition | condition | Bedingung | условие | condición |
| conic section | section conique | Kegelschnitt | коническое сечение | sección cónica |
| consequence | conséquence | Folge | следствие | consecuencia |
| consequent | conséquent | folgend; sich aus etwas
ergebend | следующий | consecuente |
| constant | constant | unveränderlich;
Konstante | постоянная | constante |
| constituent | constituant | Bestandteil | составляющий
(составляющая) | constitutivo;
constituyente |
| continued fraction | fraction continue | Kettenbruch | непрерывная дробь | cociente continuo |
| continuous function | fonction continue | stetige Funktion; kon-
tinuierliche Funktion | непрерывная функция | función continua |
| convolution | produit de composition | Faltung | свертка | convolución |
| co-prime | premiers entre eux | relativ prim | взаимно простые
(числа) | primos entre si |
| counter | compteur | Zähler; Zählrohr | счетчик | contador |
| cross-section | section | Schnitt; Querschnitt | поперечное сечение | sección recta |
| cubic equation | équation du 3 ^e degré | Gleichung drittes Grades | кубическое уравнение | ecuación cúbica |
| cursor | curseur | Läufer | ползунок | cursor |
| | | | | |
| Definite integral | intégrale définie | bestimmtes Integral | определенный
интеграл | integral definida |
| degeneracy | dégénérescence | Entartung | вырождение | degeneración |
| degenerate | dégénéré | entartet | вырожденный | degenerado |
| degree | degré | Grad | степень | grado |
| degree of freedom | degré de liberté | Freiheitsgrad | степень свободы | grado de libertad |
| denominator | dénominateur | Nenner | знаменатель | denominador |
| derivative | dérivée | Ableitung; Differential-
quotient | производная | derivada |
| desk machine | machine de bureau | Tisch- (Rechen-)
-Maschine | арифмометр | calculadora |
| determination, over- | surdétermination; cas
d'équations surabon-
dantes | Überbestimmung | сверхопределенность | superdeterminación |
| determination, under-
deviation, minimum | sous-détermination
déviation minimum | Unterbestimmung
minimale Ablenkung;
Minimalabweichung | недоопределенность
отклонение
минимальное | subdeterminación
desviación mínima |
| deviation, standard | écart normal | Streuung | отклонение
стандартное | desviación standard |
| digit | chiffre | Ziffer | цифра | dígito |
| displacement | déplacement | Verschiebung | смещение | desplazamiento |
| distribution function | fonction de répartition | Verteilungsfunktion | функция
распределения | función de distribución |
| divisor, greatest common
(g.c.d.) | diviseur, plus grand
commun (p.g.c.d.) | Teiler, grösster gemein-
samer | делитель,
наибольший общий | máximo común divisor
(m.c.d.) |
| | | | | |
| Equality | égalité | Gleichheit | равенство | igualdad |
| equation | équation | Gleichung | уравнение | ecuación |
| equidistant | équidistant | gleich entfernt (in
gleichen Abständen
befindlich) | равноотстоящий | equidistante |
| equi-inclination | équi-inclinaison | gleiche Neigung | равное наклонение | equi-inclinación |
| equivalent position | site homologue | gleichwertige Punktlage | эквивалентное
положение | posición equivalente |
| error function | fonction erreur | Fehlerverteilungsgesetz,
-funktion | кривая ошибок | función error |

9.3. DICTIONARY OF CRYSTALLOGRAPHIC TERMS

| ENGLISH | FRENCH | GERMAN | RUSSIAN | SPANISH |
|--|--|--|---|---|
| error, probable
errors, random | erreur probable
erreurs accidentelles
ou aléatoires | Fehler, wahrscheinlicher
Fehler, zufällige, oder
unsystematische | ошибка, вероятная
ошибки, случайные | error probable
errores accidentales |
| estimation
estimate, over-
estimate, under-
Eulerian cradle | évaluation
surestimation
sousestimation
berceau eulérien | Abschätzung
Überschätzung
Unterschätzung
Eulersche Aufhängung,
(Krippe) | оценка
переоценка
недооценка
« люлька » (подвеска)
Эйлера | estima
superestimado
subestimado
criba de Euler |
| evaluate
evaluation
even
example
expand; expansion
(series)
expected value | évaluer
évaluation
pair
exemple
développer; développe-
ment en série
valeur probable | auswerten
Auswertung
gerade
Beispiel
entwickeln; Entwicklung
(Reihen)
Erwartungswert | оценивать
оценка
четный
пример
расходиться,
расходимость (рядов)
ожидаемая (вероятная)
величина
погашение (погасание) | evaluar
evaluación
par
ejemplo
desarrollar, desarrollo
en serie
valor esperado o
previsto
extinción |
| extinction (absent reflec-
tion) | extinction | Auslöschung | | |
| Family (of planes)
fibre; fibrous | famille (de plans)
fibre; fibreux | Ebenenschar
Faser; faserig | семейство (плоскостей)
волокно; волокнистый
(фибриллярный) | familia (de planos)
fibra; fibroso |
| film
film pack
film shrinkage | pellicule; film
films superposés
contraction de la
pellicule ou retrait | Film
Filmpack
Schrumpfung des Films | пленка
стопка пленок
усадка пленки | película
paquete de películas
contracción de la película |
| fingerprint method | « fingerprint method » | Fingerabdruckmethode | метод отпечатков
пальца | método de huellas
dactilares |
| finite series
flat-cone method | série finie
méthode cone plat | endliche Reihe
Flachkegelmethode | конечный ряд
метод конуса с тупым
углом раствора | serie finita
método del cono plano |
| fly's-eye
fractional co-ordinates | « œil de mouche »
coordonnées fraction-
naires | „Fliegenauge“
relative Koordinaten | « мушиный глаз »
координаты в долях
периода | ojo de mosca
coordenadas
fraccionarias |
| Gear ratio | rapport des vitesses
(engrenages) | Übersetzungsverhältnis;
Getriebeübersetzung | передаточное число | reducción (engranajes) |
| grain size | granulation; taille des
grains | Korngrösse; Kristallit-
grösse | размер зерен | tamaño de grano |
| greater than (>)
group multiplication | supérieur à
multiplication sym-
bolique du groupe | grösser als
Gruppenmultiplikation | больше чем
групповое умножение | mayor que
producto de grupos |
| Hand (right, left) | sens (dextro, laevo) | Orientierungssinn
(rechts, links) | рука (правая, левая) | mano (derecha,
izquierda) |
| helical array | arrangement hélicoïdal | schraubenförmige
Anordnung | винтовое расположение | distribución helicoidal |
| helix
hindered rotator | hélice
rotateur gêné | Helix; Schraube
gehinderter Rotator | спираль
ограниченный ротатор | hélice
rotator con giro limitado |

9.3. DICTIONARY OF CRYSTALLOGRAPHIC TERMS

| ENGLISH | FRENCH | GERMAN | RUSSIAN | SPANISH |
|--------------------------------|--|--|------------------------------------|----------------------------------|
| Identity element | élément unitaire; identité | Einheitselement | единичная (тождественная) операция | elemento de identidad |
| image | image | Bild | изображение | imagen |
| improper fraction | expression fractionnaire; fraction impropre | uneigentlicher Bruch | неправильная дробь | fracción impropia |
| incompatible equations | équations incompatibles | unvereinbare Gleichungen | несовместные уравнения | ecuaciones incompatibles |
| indefinite integral | intégrale indéfinie | unbestimmtes Integral | неопределенный интеграл | integral indefinida |
| independence | indépendance | Unabhängigkeit | независимость | independencia |
| index, repeated | indice répété | Index, wiederholter | индекс, повторяющийся | indice repetido |
| inequality | inégalité | Ungleichung | неравенство | desigualdad |
| infinite | infini | unendlich | бесконечный | infinito |
| infinitesimal | infinitésimal | unendlich klein | бесконечно малый | infinitesimal |
| initial value | valeur initiale | Anfangswert | первоначальная величина | valor inicial |
| integer | nombre entier | ganze Zahl | целое число | entero |
| integrated reflection | réflexion intégrée | integrales Reflexionsvermögen; integrierte Reflexion | интегральное отражение | reflexión integrada |
| interaction | interaction | Wechselwirkung | взаимодействие | interacción |
| intercepts | coordonnées à l'origine | Achsenabschnitte | осевые единицы | segmentos interceptados |
| interchange (of rows, columns) | intervertir (rangées, colonnes) | Vertauschung (von Zeilen, Spalten) | перестановка (строк, столбцов) | intercambio (de filas, columnas) |
| interfacial angle | angle des faces | Flächenwinkel | угол между гранями | ángulo interfacial |
| interplanar distance | distance interréticulaire | Netzebenenabstand | межплоскостное расстояние | distancia interplanar; espaciado |
| intersect | se rencontrer; se couper | (sich) schneiden | пересекаться | cortar |
| intersection | point de rencontre; intersection | Schnitt | точка пересечения | intersección |
| interstice | interstice | Lücke; Zwischenraum | промежуток | intersticio |
| Kernel | noyau | Kern | ядро | núcleo |
| key result | résultat de base | aufschlussreiches Ergebnis; Hauptresultat | важнейший результат | resultado fundamental |
| knife-edge (reference) | ombre repère (de forme triangulaire) | Messerschneide; Bezugsmarke | лезвие ножа (как начало отсчета) | cuña (de referencia) |
| Lattice | réseau (réseau-période) | Translationsgitter (Gitter) | решетка | red; retículo |
| layer line | strate | Schichtlinie | слоевая линия | nivel |
| least squares | moindres carrés | kleinste Quadrate | наименьшие квадраты (чисел) | mínimos cuadrados |
| left-handed system | trièdre sinistrorsum; trièdre orienté à gauche | Linkssystem | левая система координат | sistema izquierdo |
| less than (<) | inférieur à | kleiner als | меньше чем | menor que |
| location; situation | repérage; emplacement | Ort; Lage | определение положения; локация | localización; situación |
| Magnitude | grandeur | Grösse; Größenordnung | величина | magnitud |
| matrix multiplication | multiplication matricielle | Matrizenmultiplikation | матричное умножение | producto matricial o de matrices |
| matrix notation | notation matricielle | Matrizenschreibweise | матричное обозначение | notación matricial |
| mean | moyenne | Mittel; Mittelwert; Durchschnitt | математическое ожидание | valor medio |
| mesh | maille plane | Masche | меш | trama |
| multinomial | polynôme; polynomial | polynomisch | полиномиальный | multinómico |
| multiple | multiple | vielfach | многократный | múltiple |
| multiple-exposure technique | procédé des poses multiples | Verfahren der mehrfachen Belichtung | техника многократных экспозиций | técnica de exposición múltiple |

9.3. DICTIONARY OF CRYSTALLOGRAPHIC TERMS

| ENGLISH | FRENCH | GERMAN | RUSSIAN | SPANISH |
|--|--|--|---|---|
| Neglect
net (2-dimensional lattice)
net (chart)
node (lattice, wave) | négliger
réseau plan
canevas
nœud | vernachlässigen
Translationsnetz
Netz; Diagramm
Gitterpunkt; Schwingungsknoten
Zahl; Anzahl
Zähler | пренебрегать
сетка
сетка
узел | despreciar
red
falsilla
nudo |
| number
numerator | nombre
numérateur | | число
числитель | número
numerador |
| Obliquity | obliquité | Winkelabweichung
(Zwilling); Schiefe | отклонение | inclinación |
| odd
oscillation | impair
oscillation | ungerade
Schwingung; Schwenkung | нечетный
колебание | impar
oscilación |
| Parenthesis
penultimate
perfect crystal
permitted operation
pitch (of helix)
plane
plug-board | parenthèse
pénultième
cristal parfait
opération permise
pas (de l'hélice)
plan
panneau à fiches | (runde) Klammer
vorletzt
Idealkristall
erlaubte Operation
Ganghöhe
Ebene
Schaltbrett | скобка
предпоследний
совершенный кристалл
разрешенная операция
шаг (винта)
плоскость
распределительная
доска | paréntesis
penúltimo
cristal perfecto
operación permitida
paso (de una hélice)
plano
tablero de mando |
| plus
point
port, entrance
port, exit
position
power
precision
prime (') | plus
point
fenêtre d'entrée
fenêtre de sortie
position
puissance
précision
prime | plus
Punkt
Eintrittsöffnung
Austrittsöffnung
Punktlage; Platz
Potenz
Genauigkeit
Strich | плюс
точка
вход (отверстие)
выход (отверстие)
положение, позиция
степень (мат.)
точность | más
punto
puerta de entrada
puerta de salida
posición
potencia
precisión |
| prime number
principal axis
probability
probable error
proper fraction
punched cards | nombre premier
axe principal
probabilité
erreur probable
fraction proprement dite
cartes perforées | Primzahl
Hauptachse
Wahrscheinlichkeit
wahrscheinlicher Fehler
echter Bruch
Lochkarten | простое число
главная ось
вероятность
вероятная ошибка
правильная дробь
перфорированные
карты | primo
número primo
eje principal
probabilidad
error probable
fracción propia
cartas perforadas |
| pure number | nombre pur (ou abstrait) | reine Zahl | простое число | numero puro |
| Random error | erreur accidentelle (ou aléatoire) | zufälliger (unsystematischer) Fehler | случайная ошибка | error estadístico |
| random position | position prise au hasard; | zufällige (statistische) Lage | случайное положение | posición aleatoria |
| ratio
real part
refinement (of atomic co-ordinates)
reflection; reflexion
refraction
refractive index | position quelconque
rapport
partie réelle
amélioration

réflexion
réfraction
indice de réfraction | Verhältnis
reeller Teil; Realteil
Verfeinerung;
Verbesserung
Reflexion; Spiegelung
Brechung
Brechungsindex | отношение
действительная часть
уточнение

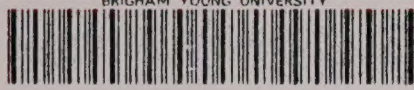
отражение
преломление
показатель
преломления | razón
parte real
refinamiento; refino;
refinado
reflexión
refracción
índice de refracción |
| relatively prime | | relativ prim | взаимно простые (числа) | primos entre si |
| repeat distance | premiers entre eux
paramètre de la rangée | Identitätsabstand;
Periode | период повторяемости | distancia de repetición |
| representation
result
right-hand rule | représentation
résultat
règle de la main droite | Darstellung
Ergebnis
Rechte-Hand-Regel;
Schraubenregel | представление
результат
правило правой руки | representación
resultado
regla de la mano derecha |
| rigorous solution | solution rigoureuse | strenge Lösung | строгое (точное)
решение | solución rigurosa |
| root mean square | racine du carré moyen | quadratischer Mittelwert* | средне квадратичный* | raiz cuadrática media |
| rotation
row line
rule
ruler | rotation
rangée réticulaire
loi
règle | Drehung
Gittergerade
Regel; Gesetz
Lineal | поворот; вращение
ряд решетки
закон
линейка | rotación
fila
ley; regla
regla |

* The German and Russian expressions include no translation of the word "root."

9.3. DICTIONARY OF CRYSTALLOGRAPHIC TERMS

| ENGLISH | FRENCH | GERMAN | RUSSIAN | SPANISH |
|---------------------------------------|---|---|--|--|
| Sample; sampling | échantillon;
échantillonnage | Probe; Probenahme | образец, проба;
опробование | muestra; muestreo |
| scale, arbitrary
scale factor | échelle arbitraire
facteur d'échelle | willkürlicher Masstab
Konversionsfaktor;
Angleichungsfaktor | шкала, произвольная
масштабный фактор | escala, arbitraria
factor de escala |
| scattering | diffusion | Streuung | рассеяние | difracción |
| screw axis | axe hélicoïdal | Schraubenachse | винтовая ось | eje helicoidal |
| sign | signe | Zeichen; Vorzeichen | знак | signo |
| simple continued fraction
(s.c.f.) | fraction continue simple | einfacher Kettenbruch | простая непрерывная
дробь | fracción continua simple |
| sinuous | sinueux | wellenförmig; gewunden;
sinusartig | извилистый | sinuoso |
| site | site | Punktlage; Platz | положение (точки) | lugar; posición |
| slide-rule | règle à calcul | Rechenschieber | логарифмическая
линейка | regla de cálculo |
| slit system | système de fentes | Spaltsystem | система расколов | sistema de ranuras |
| slope | inclinaison | Neigung | наклон | pendiente |
| solid angle | angle solide | Raumwinkel | телесный угол | ángulo sólido |
| solution (of equation) | solution | Lösung | решение | solución |
| sorting device | dispositif de triage | Sortiermaschine;
Sortiervverfahren | сортировочное
устройство | aparato de clasificación |
| space group | groupe spatial | Raumgruppe | пространственная
(федоровская) группа | grupo espacial |
| spheroid, oblate | sphéroïde aplati | abgeplattetes Sphäroid | сфероид, сжатый | esferoide oblato |
| spheroid, prolate | sphéroïde allongé | verlängertes Sphäroid | сфероид, вытянутый | esferoide prolato |
| square | carré | quadratisch | квадратный | cuadrada |
| stacking | empilement | Schichtung; Packung | наложение; упаковка | apilamiento |
| stage (of calculation) | stade (d'un calcul) | Stand (einer Rechnung) | этап (расчета) | etapa de cálculo |
| stencil | pochoir; masque | Schablone | трафарет | estarcido |
| step function | fonction en escalier | Treppenfunktion | ступенчатая функция | función de paso |
| strips | bandelettes | Streifen | штрипсы | tiras |
| superlattice | réseau multiple | Übergitter | сверхрешетка | superred |
| | | | | |
| Term | terme | Glied | член | término |
| termination (of series) | limitation (de la série) | Abbruch (einer Reihe) | обрыв (рядов) | terminación de serie |
| trace | trace | Spur | след | traza |
| trial | essai | Versuch | проба | tanteo |
| trial and error | essais et retouches | „trial and error“;
systematisches
Probieren | проб и ошибок (метод) | método de tanteo |
| | | | | |
| triangle; triangular | triangle; triangulaire | Dreieck; dreieckig | треугольник;
треугольный | triángulo; triangular |
| twin | macle | Zwilling | двойник | macla; geminación |
| | | | | |
| Uncertainty | incertitude | Unsicherheit;
Unbestimmtheit | неопределенность | incertidumbre |
| unique | unique | einzig; eindeutig | единственный | único |
| unknown | inconnu | unbekannt | неизвестный | desconocido |
| upper layer | strate supérieure | obere Schicht; Ober-
schicht | верхний слой | estrato (nivel) superior |
| | | | | |
| Variable | variable | veränderliche Grösse | переменный | variable |
| vertex | sommet | Scheitel | вершина | vértice |
| void | trou; vide; lacune | Lücke; leer; nichtig | пустота | hueco |
| | | | | |
| Weight (of observation) | poids | Gewicht | вес | peso |
| | | | | |
| Zero | zéro | Null | нуль | cero |

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